Abstract

Numerical calculations of the valence band and conduction band size quantized levels in a strained \( p-Al_{x}Ga_{1-x}As/GaAs_{1-y}P_{y}/n-Al_{x}Ga_{1-x}As \) \( (y = 0.16) \) double heterostructure were performed for different values of the external uniaxial compression along the [110] direction. They indicate that the two upper levels in the valence band—light hole LH1 and heavy hole HH1—intersect at a pressure of about 4 kbar, and a strong LH1-HH1 state mixing develops around the crossover point. The results of calculations explain the nonlinear character of the photon energy shift and electroluminescence intensity increase that were experimentally observed in these structures under uniaxial compression up to 5 kbar.

1. Introduction

In recent decades, hydrostatic pressures and uniaxial compression have been used as a strong external influence on the band structure and energy spectrum of charge carriers in solids leading to their quantitative and qualitative reconstruction. In particular, metal–insulator transitions have been observed in some materials [1] as well as a range of electronic topological transitions in BiSb alloys [2]. The last time, the possibility to change the wavelength of laser diodes by means of external uniaxial stress [3] and uniform compression in hydrostatic pressure chambers [4, 5] has been successfully demonstrated. The method of uniaxial compression, which was described previously in [6], is more convenient for optical measurements in comparison with hydrostatic pressure cells, because it allows a free withdrawal of radiation from a sample for a spectral analysis. It was developed in combination with an optical cryostat of a simple construction that may be produced in a laboratory workshop.

It was shown [3] that, under uniaxial compression up to \( P = 4 \) kbar in the [110] and [1-10] directions, the electroluminescence (EL) spectra of strained \( p-Al_{x}Ga_{1-x}As/GaAs_{1-y}P_{y}/n-Al_{x}Ga_{1-x}As \) \( (y = 0.16) \) double heterostructures, which are usually used in TM emitting 808-nm high-power diode lasers, exhibit a blue shift, while the EL intensity shows a 2-3 times increase. The photon energy shift in respect to the applied stress is not linear and determined by the increase in the energy gap in the quantum wall (QW) material under compression, but the enhancement of the EL intensity remained uncertain and cannot be explained either by decrease of non-radiative recombination under compression or by arising piezoelectric field or a potential barrier lowering. (a) Non-radiative Auger-recombination is not essential in a wide-gap GaAs_{0.84}P_{0.16} QW with an energy gap of about 1.616 eV that only increases under compression. (b) In these structures, the piezoelectric field arises in opposite directions under uniaxial compression applied along the [110] and [1-10] axes, while the effect of EL intensity increase is the same in both cases. (c) According to the calculations [7], the lowering
of the potential barriers under compression, which can cause the increase of the injected currents into the QW, is not more than 3% and cannot explain 2-3 times increase in the EL intensity.

In this research, we have extended the pressure interval of the EL study up to $P = 5 \text{kbar}$ and search for the explanation of the intensity increase under compression in the shifts of heavy hole and light hole eigenenergies in the biaxially strained GaAs$_{0.84}$P$_{0.16}$ QW that could result in the mixing of valence band states and a change in transition probabilities.

2. Experimental details and results

The studied $p$-Al$_{x}$Ga$_{1-x}$As/GaAs$_{1-y}$P$_{y}$/n-Al$_{x}$Ga$_{1-x}$As ($y = 0.16$) structures were grown on silicon doped (001) GaAs substrates by metal organic vapor-phase epitaxy. A GaAs$_{0.84}$P$_{0.16}$ QW of a 14 nm width is surrounded on both sides by Al$_{0.45}$Ga$_{0.55}$As waveguide barrier layers of 1-$$\mu m$$ thickness with various $p$- and $n$-types levels of doping, which, starting from $1 \times 10^{17} \text{ cm}^{-3}$ near the QW, reaches $2 \times 10^{18} \text{ cm}^{-3}$ in the peripheral areas of the structure. It is essential that, due to the mismatch of the crystal lattice parameters, the QW is under a biaxial stretched strain of 0.58% arising in the process of the epitaxial growth. Due to this strong built-in strain of the QW material, the ground state of light holes (LH1) appears in the energy scale over the ground state of heavy holes (HH1).

The EL spectra were recorded by using an automated unit consisting of a personal computer and an MDR-12 monochromator, which provides accuracy in measurements with a dispersion of 2.4 nm/mm. When the width of the entrance slot is less than 30 $\mu m$, it allows a spectral resolution of up to 0.1 nm, which corresponds to the determination accuracy of the photon energy 0.3–0.4 meV in the visible and near infrared spectral regions. Measurements can be performed with a constant step of wavelength $\Delta L = 0.1–1 \text{ nm}$ with up to 170–1700 points on the spectral range averaged over 1–25 measurements at each point. The digital devices used in the measurement system for the amplification and measurement of signals allow increasing the dynamic range by up to five orders of magnitude. The EL spectra were investigated at currents through the diode in the range of 0.1–30 mA. Current was normal to the plane of the structure, and the light emission was perpendicular to the direction of compression.

![Fig. 1](image1.png)

Fig. 1. EL spectra measured at 77 K under uniaxial compression along the [110] axis in the $p$-Al$_{x}$Ga$_{1-x}$As/GaAs$_{1-y}$P$_{y}$/n-Al$_{x}$Ga$_{1-x}$As ($y = 0.16$) heterostructure. Insert: the pressure dependence of the photon energy shift.

![Fig. 2](image2.png)

Fig. 2. Spectra of TM-mode (1, 2) and TE-mode (3, 4) measured at a temperature of 77 K under uniaxial compression along the [110] direction.
Applied stress limit was increased in this work from 3.9 kbar [6] up to 5.1 kbar by successful compression of thinner samples. The EL spectra measured at 77 K and forward current 5.5 mA (Fig. 1) indicate the same nonlinear blue shift and EL intensity increase that were detected in [6] under uniaxial compression up to 3.9 kbar. The maximal shift of EL photon energy at $P = 5.1$ kbar is about 30 meV.

The effect of uniaxial stress influence on EL polarization is represented in Fig. 2. It indicates the relative decrease of TE-mode under compression in respect to TM-mode: the intensity ratio $I_{TE}/I_{TM} = 1.4$ at $P = 0$ decreases up to $I_{TE}/I_{TM} = 1.2$ at $P = 5.1$ kbar. The data in Figs. 1 and 2 are representative of the significant change in the energy band structure and size quantized level states in the QW under uniaxial stress that are calculated and analyzed in the next section.

3. Numerical calculations and discussion

The valence band and conduction band size quantized levels, as well as wave functions of electrons and holes, in the investigated GaAs$_{0.84}$P$_{0.16}$ QW were numerically calculated for different values of the external uniaxial compression along the [110] direction. The Luttinger-Kohn Hamiltonian with strain terms was self-consistently solved together with the Poisson equation for the electrostatic potential using the finite-difference $k\cdot p$ method in the framework of the model developed in [8]. The necessary parameters were taken from the literature [9].

According to the calculations, in the strained GaAs$_{0.84}$P$_{0.16}$ QW under investigation at $P = 0$, the LH1 level is the ground state in the valence band, while the HH1 level is the next one in the energy scale. Optical transitions between the lowest electron level $e_1$ and the highest hole level in the valence band determine an optical gap that is equal to the experimentally observed emitted photon energy.

Under uniaxial compression, LH1 and HH1 levels move toward each other and, after $P \sim 4$ kbar, the HH1 becomes the hole ground state in the GaAs$_{0.84}$P$_{0.16}$ QW (Fig. 3). The crossover of LH1 and HH1 levels naturally explains the nonlinear character of the optical energy gap shift under an applied uniaxial stress. It is represented in Fig. 4 together with the experimental data.

![Fig. 3. Calculated energy shifts of light (LH1, LH2) and heavy (HH1, HH2, HH3) hole states under uniaxial compression along the [110] direction.](image1)

![Fig. 4. Calculated pressure dependence of the optical energy gap shift. Dots are experimental data obtained for different samples.](image2)
In calculations, the hole wave functions were expanded in basis functions of the Lattinger-Kohn representation with the total angular momentum $J = 3/2$, and its projections $m_J = \pm 1/2$ and $m_J = \pm 3/2$ correspond to light holes and heavy holes, respectively, in the absence of strain [8]. Analysis of the envelope functions related to the two upper levels in the valence band QW LH1 and HH1 permit evaluating the input from the basis functions with different total angular momentum projection into the light and heavy hole wave functions under uniaxial compression. The results depicted in Fig. 5 indicate that at $P = 0$ light holes are described only by basis functions with $|m_J| = 1/2$; heavy holes, by basis function with $|m_J| = 3/2$. The picture demonstrates the development of mixing of light hole and heavy hole states under compression and LH1-HH1 crossover.

![Fig. 5. Pressure dependence of relative input of basis functions with different angular momentum projection $|m_J| = 3/2$ (1) and $|m_J| = 1/2$ (2) into wave functions of (a) heavy and (b) light hole ground states.]

From electron and hole wave functions, matrix elements of electron-photon interaction operator for interband transitions and, further, absorption coefficient and optical gain can be calculated [10]. Optical gain spectra for TM- and TE-modes of polarized light are represented for different values of applied stress in Fig. 6. The electron and hole concentration in the QW $n = p = 2 \times 10^{12}$ cm$^{-2}$, that is characteristic of the used range of currents, was taken in calculations. Corresponding to the geometry of the experiment, electromagnetic wave propagation was assumed to be along the structure in the [1-10] direction that is perpendicular to the stress applied in the [110] direction.

The TM-mode optical gain represented in Fig. 6 demonstrates the significant increase under compression up to 8 kbar in a wide photon energy range. The transformation of TE-mode optical gain is complicated: it increases at low stress and drops at $P > 4$ kbar. These results of numerical calculations are qualitatively consistent with experimentally observed effects: (1) 2-3 times increase in the EL intensity under compression up to 5 kbar (Fig. 1) and (2) a decrease in the relative light polarization at high pressures (Fig. 2).

The increase in the optical gain under uniaxial compression is evidently connected with the LH1-HH1 crossover at $P_c \approx 4$ kbar that determines the increase in the joint hole density of states due to higher value of the heavy hole effective mass in comparison with the light hole one. Since the mixing of heavy hole and light hole states develops in a definite pressure interval (Fig. 5), in this region of pressure, there exists a noticeable mixing of their wave functions and, as a result, selection rules soften and optical transition probability increases. The degree of mixing depends
on the energy splitting of LH1 and HH1 levels around the merger point $P_c$. On the average, this situation leads to a smooth increase in the EL intensity under compression in the vicinity of $P_c$ point. After $P_c$ EL intensity increment is still possible due to high density of heavy hole states. It is remarkable that the nonlinear behavior of the optical energy gap starts to be evident at pressure $P \approx 2$ kbar (Fig. 3) where the LH1-HH1 state mixing begins (Fig. 5).

![Fig. 6. Transformation of optical gain spectra of TM-mode (a) and TE-mode (b) under compression along the [110] direction.](image)

It should be noted that the valence band mixing was studied previously mainly in a series of experiments where the shift of light and heavy hole levels in the QW depending on internal biaxial strain was regulated either by the QW and the barrier composition [11] or by etching of the substrate [12]. An enhancement in exitonic absorption due to the overlap in heavy-hole and light-hole exitons was detected in [12]. In this work, the development of the mixing of light and heavy hole wave functions was investigated for the same sample in the course of one experiment, which makes the observed phenomenon of EL intensity increase under uniaxial compression highly reliable.

4. Conclusions

It is shown that, under uniaxial compression up to 5 kbar, the EL spectra of strained $p$-Al$_x$Ga$_{1-x}$As/GaAs$_{1-y}$/n-Al$_x$Ga$_{1-x}$As ($y = 0.16$) double heterostructures demonstrate a nonlinear blue photon energy shift and a 2-3 times increase in the EL intensity. The effect of uniaxial stress on EL polarization results in a relative decrease in the TE-mode in respect to the TM-mode under compression: $I_{TE}/I_{TM} = 1.4$ at $P = 0 \rightarrow I_{TE}/I_{TM} = 1.2$ at $P = 5.1$ kbar.

Numerical calculations of the $p$-Al$_x$Ga$_{1-x}$As/GaAs$_{1-y}$/n-Al$_x$Ga$_{1-x}$As ($y = 0.16$) band structure and size quantized levels in the QW under uniaxial stress indicate a LH1-HH1 crossover at a pressure of about 4 kbar that determines a nonlinear increase of the optical gap magnitude and accordingly EL photon energy. The input of LH1 and HH1 states into light emission is calculated and analyzed: the development of strong LH1-HH1 mixing around the crossover point and transition of the hole ground state in the QW from LH1 ($|m_J| = 1/2$) to HH1 ($|m_J| = 3/2$) are shown. Matrix elements of the electron-photon interaction Hamiltonian and optical gain were calculated for different polarizations (TE and TM-modes). The result indicates the increase in the intensity of these modes in the vicinity of the LH1–HH1 crossover as well as its relative change under conditions of LH1–HH1 mixing.
References