Uniaxial compression influence on valence sub-bands energy spectrum and electroluminescence in n-AlGaAs/GaAsP/p-AlGaAs diode structures

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Abstract. Numerical calculations of the valence band and conduction band size quantized levels in a strained $p$-$\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}_{1-y}\text{P}/n$-$\text{Al}_x\text{Ga}_{1-x}\text{As}$ ($y = 0.16$) double heterostructure were performed for different values of the external uniaxial compression along $[110]$ direction. They indicate that the two upper levels in the valence band merge at pressure about 4 kbar and a strong state mixing develops around the merging 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
For a long time hydrostatic pressure and uniaxial compression were 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. Recently, the possibility to change the wavelength of laser diodes by means of external uniaxial stress [1] and uniform compression in hydrostatic pressure chambers [2] has been successfully demonstrated. The method of uniaxial compression used in [1] up to pressure $P = 4 - 5$ kbar is more convenient for optical measurements, because it allows a free withdrawal of radiation from a sample for a spectral analysis.

It has been shown [1] that under uniaxial compression in $[110]$ and $[1-10]$ directions electroluminescence (EL) spectra of strained $p$-$\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}_{1-y}\text{P}/n$-$\text{Al}_x\text{Ga}_{1-x}\text{As}$ ($y = 0.16$) double heterostructures usually used in TM emitting 808 nm high-power diode lasers demonstrate a blue shift, while the electroluminescence intensity shows 2 - 3 times increase (figure 1). Moreover, the effect of uniaxial stress influence on EL polarization (figure 2) indicates the relative decrease of TE-mode under compression in respect to TM-mode. The photon energy shift in respect to the applied stress is not linear (see insert in figure 1) and determined by increase of the energy gap in quantum well (QW) material under compression, but the enhancement of the EL intensity remained uncertain and can not be qualitatively explained either by decrease of nonradiative recombination under compression or by arising piezoelectric field or a potential barrier lowering.

The present paper is aimed on the numerical calculations and analysis of the energy spectrum in $p$-$\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}_{1-y}\text{P}/n$-$\text{Al}_x\text{Ga}_{1-x}\text{As}$ ($y = 0.16$) diode structure under uniaxial compression, since the EL data described above [1] (see figures 1, 2) are representative of the significant change in the energy band structure and size quantized level states in the QW under uniaxial stress.
2. Numerical calculations and discussion

The $p$-$Al_{x}Ga_{1-x}As/GaAs_{1-y}P/n-Al_{x}Ga_{1-x}As$ ($y = 0.16$) structures under investigations 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 micron thickness on the whole with various $p$- and $n$-types levels of doping, which, starting from $1 \times 10^{17}$ cm$^{-3}$ near the QW, reaches $2 \times 10^{18}$ cm$^{-3}$ in the peripheral areas of the structure.

The valence and conduction band profiles, as well as size quantized levels and 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 [110] direction. The Luttinger-Kohn Hamiltonian with strain terms [3] was self-consistently solved together with Poisson’s equation for the electrostatic potential using the finite-difference $k \cdot p$ method. Numerical calculations were performed in the framework of the program “Heterostructure Design Studio 2.1” in the vicinity of the zone centre at the $\Gamma$ point. There was used the model developed in [4], which considers the Luttinger-Kohn Hamiltonian 6x6 and describes the conduction band, light and heavy hole subbands but doesn’t take into account the valence split-off subband lying about 300 meV below the top of the valence band in GaAs$_{0.84}P_{0.16}$ [5]. Necessary for calculations parameters were taken from literature [5].

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 valence band while the heavy hole HH1 level is the next one in the energy scale (figure 3). Optical transitions between the lowest electron level e1 and the highest hole level h1 in the valence band determine an optical gap that is equal to the experimentally observed emitted photon energy and increases with applied stress. Under uniaxial compression levels h1 and h2 move toward each other, and their merging with the following repulsion takes place at $P \approx 4.5$ kbar (figure 3). As soon the transitions from the electron level e1 to the uppermost hole level h1 dominate in EL, the h1-h2 exchange in the character of the pressure dependence after the merging can explain the observed nonlinearity in the EL photon energy shift (see figure 4).

In calculations, the hole wave functions were expanded in basis functions of Luttinger-Kohn representation with the total angular momentum $J = 3/2$, and its projections $m_0 = \pm 1/2$ and $m_1 = \pm 3/2$ correspond to light holes and heavy holes respectively [4]. Applied uniaxial stress reduces the symmetry and causes the hole state mixing. Analysis of the envelope functions related to the two upper levels in the valence band QW permits to evaluate the contribution of the basis functions with different total angular momentum projections into the wave functions on h1 and h2 levels under uniaxial compression. The results depicted in figure 5 indicate that at $P = 0$ light holes (LH1 state, h1 level) are described only by basis functions with $|m_0| = 1/2$, while heavy holes (HH1 state, h2 level) – by basis function with $|m_0| = 3/2$. The picture demonstrates the development of light hole – heavy hole states mixing under compression and LH1-HH1 states merging at $P \approx 4$ kbar.
From the electron and hole wave functions matrix elements of electron-photon interaction operator for interband transitions and, further, absorption coefficient and optical gain may be calculated [6]. Optical gain spectra for TM- and TE-modes of polarized light are represented in figure 6 for different values of applied stress. In calculations, electron and hole concentration in QW was taken to be \(n = p = 2 \times 10^{12} \text{ cm}^{-2}\) that is characteristic for the used range of currents. The TM-mode optical gain represented in figure 6 demonstrates significant increase under compression up to 8 kbar in a wide photon energy range. 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 EL intensity increase under compression (see figure 1) and (2) decrease of relative light polarization at high pressures (see figure 2).

The increase of the optical gain under uniaxial compression is evidently connected with the LH1-HH1 merging at \(P \approx 4\) kbar that determines growing of the joint hole density of states due to the higher value of the heavy hole effective mass in comparison with the light hole one. Since the strong mixing of heavy hole and light hole states develops in a definite pressure interval (figure 5), in this region of pressure there exists a noticeable mixing of their wave functions and, as a result, selection rules “softening” and optical transition probability enhancement. The degree of mixing depends on the h1 and h2 levels splitting \(\Delta\). This situation leads to a smooth EL intensity increase under compression in the vicinity of \(\Delta \approx 0\). At \(P \geq 4\) kbar EL intensity increment is still possible due to the high density of heavy hole states. It is remarkable that non-linear behavior of optical energy gap starts to be evident at pressure \(P \approx 2\) kbar (figure 4) where the strong LH1-HH1 state mixing begins (figure 5).

It should be noted, that the valence band mixing was studied previously mainly in a series of experiments with different samples, and the shift of light and heavy hole levels in QW in dependence on the internal biaxial strain was regulated by QW and barrier constitution [7]. In [1] the development

**Figure 3.** Calculated energy shifts of five upper (h1-h5) hole levels at \(\Gamma\) point under uniaxial compression along [110] direction.

**Figure 4.** Calculated pressure dependence of the optical energy gap shift. Dots – experimental data obtained for different samples.

**Figure 5.** Relative contribution of basis functions with different angular momentum projections \(|m_J| = 3/2 (1)\) and \(|m_J| = 1/2 (2)\) into wave functions of holes on h1 (a) and h2 (b) levels under uniaxial compression.
of light and heavy hole wave functions mixing process was investigated on the sample in the course of one experiment that makes the observed phenomenon of EL intensity increase under uniaxial compression single-valued and highly reliable.

3. Conclusion

The experimental data on EL spectra of strained \( p-Al_{x}Ga_{1-x}As/GaAs_{1-y}P/n-Al_{x}Ga_{1-x}As \) (\( y = 0.16 \)) diode structures under compression up to 4 - 5 kbar [1] demonstrated a nonlinear blue photon energy shift, 2 - 3 times increase of EL intensity and relative decrease of TE-mode in respect to TM-mode under compression, that are representative of a significant change in the energy band structure.

Numerical calculations of the \( p-Al_{x}Ga_{1-x}As/GaAs_{1-y}P/n-Al_{x}Ga_{1-x}As \) (\( y = 0.16 \)) band structure and size quantized levels in QW under uniaxial stress performed in the present paper indicate a merger of two uppermost hole levels (LH1-HH1 states) at pressure about 4 kbar that determines nonlinear increase of the optical gap magnitude and correspondently EL photon energy. Development of strong LH1-HH1 mixing and transition of the hole ground state in the QW from LH1 nature (\(|m_J| = 1/2\)) to HH1 nature (\(|m_J| = 3/2\)) 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 increase of these modes intensity in the vicinity of LH1–HH1 merging as well as its relative change under condition of LH1–HH1 mixing.

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Figure 6. Optical gain spectra of TM-mode (a) and TE-mode (b) under compression along [110] direction.