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Temperature and Deformation Dependence of *p*-$Al_xGa_{1-x}As/GaAs_{1-y}P_y$/*n*-$Al_xGa_{1-x}As$ Laser Diode Wavelength and Polarization

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Numerical calculations of the optical energy gap and the optical gains g_{TE}, g_{TM} of TE and TM polarization modes in *p*-$Al_xGa_{1-x}As/GaAs_{0.84}P_{0.16}$/*n*-$Al_xGa_{1-x}As$ laser diode structure are carried out for uniaxial compression up to $P = 10$ kbar along in-plane and normal to a heterostructure directions at temperature interval 77 K – 300 K. The optical energy gap shift under compression is substantially anisotropic and does not change significantly between 77 K and 300 K. The g_{TM}/g_{TE} ratio is also almost insensitive to the temperature but demonstrates several times decrease under in-plane compression and no change under compression normal to a heterostructure.

1. Introduction

The results of this paper mainly concern the packaging-induced strain that might be caused in AlGaAs based laser devices by their soldering to a heat sink and, as well, the strain influence on the performance properties. Previously, strong effects of anisotropic stress on wavelength and polarization of the $A^{III}B^{V}$ based semiconductor diode lasers emission were detected and investigated, for example by producing a bending stress in InGaAsP semiconductor laser chips [1]. With development of semiconductor laser technique, packaging-induced strains, as well as possible anisotropic stress influence on the emitted light characteristics, were studied both by direct spectroscopic measurements [2,3] and quantitative strain analysis [4].

In our recent papers [5,6] systematic experimental study and numerical calculations of external uniaxial compression P influence on the energy spectrum, wave functions, and the optical gain g_{TE}, g_{TM} of TE and TM polarization modes in *p*-$Al_xGa_{1-x}As/GaAs_{1-y}P_y$/*n*-$Al_xGa_{1-x}As$ laser diode structures of different quantum well (QW) thickness and composition were performed for temperature $T = 77$ K and $P \parallel [110]$ direction. According to the experimental study [6], under [110] uniaxial compression ($P \approx 5$ kbar) the electroluminescence spectrum in *p*-$Al_xGa_{1-x}As/GaAs_{0.84}P_{0.16}$/*n*-$Al_xGa_{1-x}As$ laser diodes demonstrates a blue shift up to 25 meV, while the intensity of light in the plane normal to the heterostructure reveals not only the strong increase under compression in [110] direction, but also evident decrease of relative TM/TE intensity ratio. Very good agreement between numerical calculations and experimental results for the structure with $GaAs_{0.84}P_{0.16}$ quantum well of 14 nm width under uniaxial compression along [110] direction makes the results of numerical calculations for *p*-$Al_xGa_{1-x}As/GaAs_{1-y}P_y$/*n*-$Al_xGa_{1-x}As$ laser diode structures, performed with other QW compositions, thickness, and other directions of applied stress, quite reliable.

Taking into account that laser diodes operate actually at about room temperature and mechanical strains, introduced by their soldering [7] on a heat sink, may arise in different directions, we performed also in this work the results of analogous calculations, carried out for compression up to $P = 10$ kbar along [100] and [001] directions (in-plane and normal to a heterostructure) at 77 K and

300 K, shown together with the previous results [5,6].

2. Numerical Calculations

Numerical calculations of uniaxial stress influence on the energy spectrum, wave functions, matrix elements of electron-photon interaction operator as well as the optical gain of TE and TM polarization modes in strained p-$Al_xGa_{1-x}As/GaAs_{1-y}P_y/n$-$Al_xGa_{1-x}As$ laser diode structures have been performed for the experimentally investigated in Refs. [5,6] structure with $GaAs_{0.84}P_{0.16}$ QW of 14 nm width under uniaxial compression up to 10 kbar along [110], [100], and [001] directions at 77 K and 300 K. The Luttinger-Kohn Hamiltonian with strain terms [8] was self-consistently solved together with Poisson's equation for the electrostatic potential using the finite-difference $\mathbf{k}\cdot\mathbf{p}$ method. Numerical calculations were fulfilled in the framework of the program "Heterostructure Design Studio 2.1" in the vicinity of the zone centre at the Γ point. There was used the model developed in Ref. [9], which considers the Luttinger-Kohn Hamiltonian 6×6 and describes the conduction band, light and heavy hole subbands but doesn't take into account the valence spin-off subband lying about 300 meV below the top of the valence band in $GaAs_{0.84}P_{0.16}$ [10].

In the calculations, both external and internal strain effect were considered. Internal strains arising because of lattice mismatch of layers in zinc blend $A^{III}B^{V}$ heterostructures grown in [001] direction are described by nonzero tensor components:

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_0 - a}{a}; \qquad \varepsilon_{zz} = \frac{2C_{12}}{C_{11}} \varepsilon_{xx} , \qquad (1)$$

where a_0 and a are the lattice constants of the substrate and the layer; C_{11} and C_{12} are the stiffness constants [10]; x, y, z are determined by the crystallography directions [100], [010] and [001] correspondently.

Nonzero strain tensor components corresponding to the external uniaxial compression in [110], [100] and [001] directions are represented by following expressions [9]:

$$\begin{aligned} &\varepsilon_{xx} = \varepsilon_{yy} = \frac{S_{11}+S_{12}}{2} P, \quad \varepsilon_{zz} = S_{12}P, \quad \varepsilon_{xy} = \frac{S_{44}}{4} P \quad \text{for } P \parallel [110], \\ &\varepsilon_{xx} = S_{11}P, \quad \varepsilon_{yy} = \varepsilon_{zz} = S_{12}P \quad \text{for } P \parallel [100], \qquad (2) \\ &\varepsilon_{xx} = \varepsilon_{yy} = S_{12}P, \quad \varepsilon_{zz} = S_{11}P \quad \text{for } P \parallel [001], \end{aligned}$$

where S_{11}, S_{12}, S_{14} are elastic modulus. The total strain is described by the sum of the corresponding components from (1) and (2).

The used program provides also the possibility of calculations for different values of temperature T, and the lattice constant in this case is [10]:

$$a(T) = a(300) + a_T(T - 300),$$

where $a(300)$ is the value at $T = 300$ K and a_T is the coefficient of the linear temperature expansion. According to the empirical expression [10], the energy gap is:

$$\varepsilon_g(T) = \varepsilon_g(0) - \frac{\alpha T^2}{T + \beta},$$

where α and β are the fitting parameters, $\varepsilon_g(0)$ is the energy gap at $T = 0$.

The other necessary for calculations parameters were taken from literature [10]. For more details of numerical calculations and experimentally investigated samples see Ref. [5].

3. Results and Discussion

The results of calculations for P ‖ [100] and P ‖ [001] together with the previous data for P ‖ [110] are represented in Fig. 1. The emitted light wavelength is determined by the optical gap E_{opt} that is equal to the difference of the energies of the electron and hole ground states in a quantum well. In the temperature interval under consideration E_{opt} increases and $\Delta E_{opt} \approx 77$ meV. In comparison with this value, its shift under compression is moderate and does not change between 77 K and 300 K, but substantially anisotropic (Fig. 1a). This $\Delta E_{opt}(P)$ temperature behavior is explained by the absence of deformation potentials dependence on temperature and very low temperature dependence of elastic modulus [11]. From the other side, the results show that polarization of emitted light can be extremely sensitive to external uniaxial stress (see Fig. 1b) due to the change of wave functions and optical transitions between the subband levels in the quantum well [5,6]. If P ‖ [110] (or P ‖ [100]) the increase of applied uniaxial compression leads to the strong change of the energy spectrum of light (LH) and heavy (HH) holes (Fig. 2) [5]. At zero external compression the uppermost level h1 and the next level h2 are pure LH states, at the same time the level h3 is a pure HH state. While the compression increases the HH state is admixed to LH ones. Finally the share of HH state becomes even dominant on the level h2 and it becomes almost of HH nature (Fig. 2c). These changes in the topmost states of the QW remove the prohibition on the interband transitions to occur only in the TM mode.

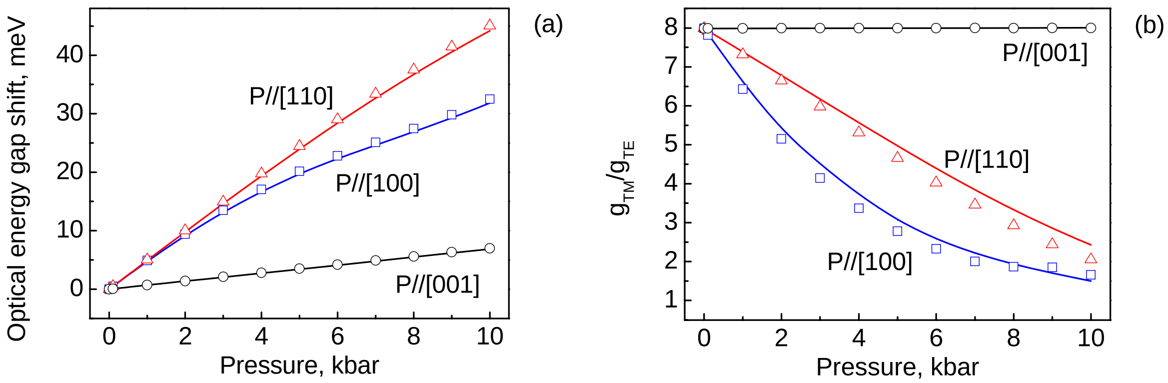

Fig. 1. Pressure dependence of the optical energy gap (a) and g_{TM}/g_{TE} ratio (b) for the $GaAs_{0.84}P_{0.16}$ QW of 14 nm width under uniaxial compression along different directions at $T = 77$ K (lines) and $T = 300$ K (symbols).

The results of calculations for the experimentally investigated laser diode structure [5] demonstrates (Fig. 1b) that in the 14 nm quantum well with phosphorus fraction of 0.16 the ratio g_{TM}/g_{TE} of optical gain in the TM and TE modes at zero compression is equals to about 8. Under compression $P = 5$ kbar in [110] direction the g_{TM}/g_{TE} ratio strongly drops to approximately 5, i.e. in 1.6 times, that is in a good agreement with the experimental data on decrease of relative TM/TE intensity ratio with about 5% of variance [6]. This agreement supports calculations performed for the other stress directions in the framework of the program “Heterostructure Design Studio 2.1”. Even more strong decrease reveals g_{TM}/g_{TE} ratio in the case of compression along in-plane [100] direction (Fig. 1b). The g_{TM}/g_{TE} ratio does not show any change under compression along [001] because, being perpendicular to the heterostructure, uniaxial compression in this direction does not influence on the wave function symmetry. The fact that under in-plane compression g_{TM}/g_{TE} ratio shows noticeable decrease even at moderate uniaxial stress and a small temperature dependence indicates, that p-$Al_xGa_{1-x}As/GaAs_{1-y}P_y/n$-$Al_xGa_{1-x}As$ structures can be used in devices for TM – TE modes switching and, as well, for stress detection and characterization.

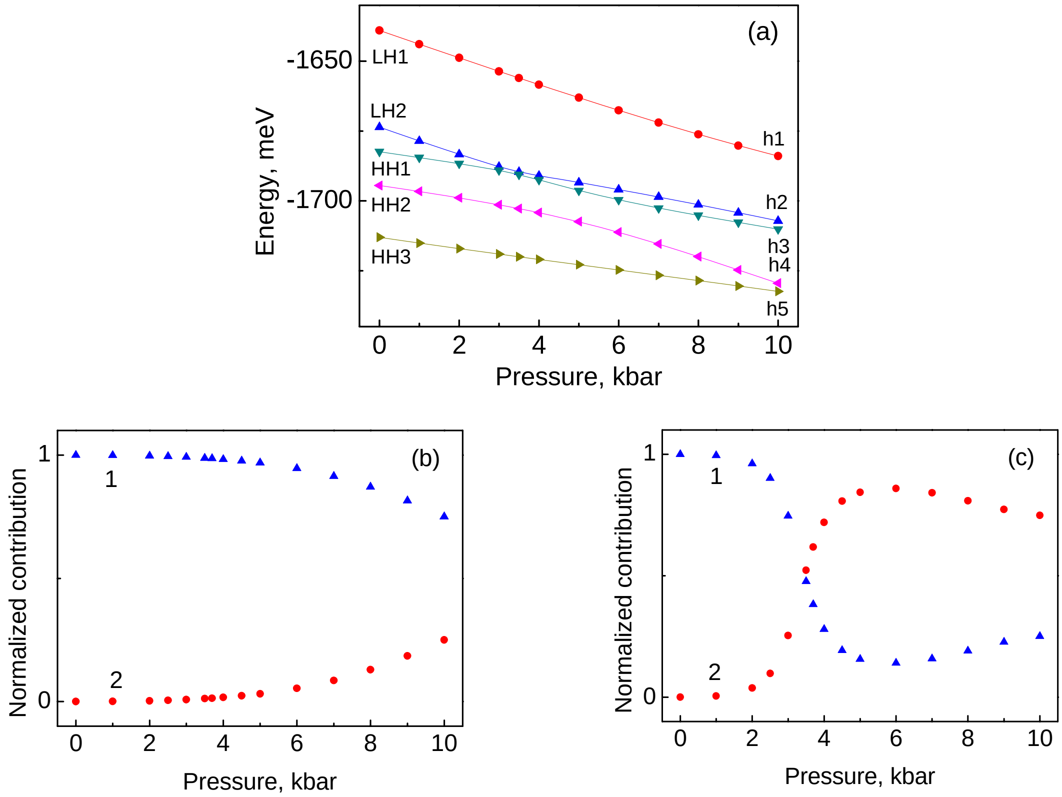

Fig. 2. Calculated energy shifts of five hole levels at the zone center under uniaxial compression (a) and pressure dependence of normalized contribution of basis functions with different angular momentum projection $|m_J| = 1/2$ (1) and $|m_J| = 3/2$ (2) into wave functions of h1(b) and h2 (c) hole levels for the $GaAs_{0.84}P_{0.16}$ QW of 14 nm width ($P \parallel [110]$, $T = 77$ K) [5].

For the laser diode heterostructures under consideration: $GaAs_{0.84}P_{0.16}$ QW of 14 nm width – the reverse of the external strain from compression to tension leads to the reversed dependence of the optical gap and g_{TM}/g_{TE} ratio on strain (Fig. 3). Nevertheless, the demonstrated in Fig. 3 linearity of these effects in a rather wide interval of pressure is not universal, and for structures with other quantum wells may be determined by the energy spectrum of heavy and light holes and works only in the vicinity of $P = 0$.

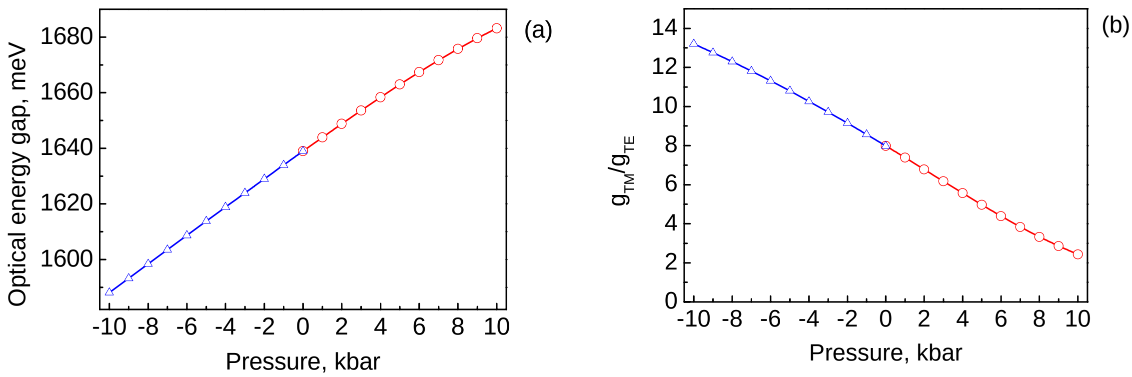

Fig. 3. Pressure dependence of the optical energy gap (a) and g_{TM}/g_{TE} ratio (b) for the $GaAs_{0.84}P_{0.16}$ QW of 14 nm width under uniaxial compression (circles) and tension (triangles) along [110] direction at $T = 77$ K.

4. Conclusion

In this paper we have presented the results of numerical calculations of uniaxial stress influence on the optical gap and TM-TE polarization modes intensity in *p*-$Al_xGa_{1-x}As/GaAs_{0.84}P_{0.16}$/*n*-$Al_xGa_{1-x}As$ laser diode structure usually used in TM emitting 808 nm high-power semiconductor lasers. The calculations are performed under compression up to 10 kbar along the main in-plane [110], [100] and normal to the heterostructure [001] crystallography directions in the temperature interval 77 K – 300 K. They indicate that the most effective blue shift of the emission spectrum is possible under compression in [110] direction. At the same time, the optical gain g_{TM}/g_{TE} ratio reveals strong several times decrease under in-plane [110] and [100] compression and, as it was shown previously [6], this effect may be specially increased in *p*-$Al_xGa_{1-x}As/GaAs_{1-y}P_y$/*n*-$Al_xGa_{1-x}As$ structures by the proper choice of quantum well thickness and composition. In this aspect, some devices for effective TM and TE polarization modes tuning and switching under uniaxial stress based on *p*-$Al_xGa_{1-x}As/GaAs_{1-y}P_y$/*n*-$Al_xGa_{1-x}As$ laser diode structures are possible. As it have been already mentioned, the performed calculations are also useful to anticipate and evaluate mounting and temperature induced strain effects on the diode laser performance and, quite the reverse, the detected shifts in parameters of laser emission may be applied for analysis of the arising strain. It should be mentioned that the demonstrated numerical calculations in the framework of the program "Heterostructure Design Studio 2.1" can be applied to other layered quantum well structures of zinc blend $A^{III}B^{V}$ semiconductor materials that are base for the modern optoelectronics.

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