Pressure-Driven Reordering of Valence Band States in AlGa_N/AlN Quantum Wells

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We study theoretically the influence of external hydrostatic pressure on the valence band structure in [0001]-oriented Al_xGa_{1-x}N/AlN quantum wells used in deep-ultraviolet light emitting devices. The calculations performed using the multi-band $k \cdot p$ method with excitonic effects show that for Al_xGa_{1-x}N/AlN quantum wells with $x = 0.7$ and quantum well width of 1.5 nm, reordering of the topmost valence subbands having different symmetries occurs with increasing pressure. In these structures, at low pressure values the topmost valence level is of Γ_9 symmetry whereas it changes to the Γ_7 state for pressures about 2.5 GPa. We also find that the excitonic effects increase the critical value of pressure at which the change in the polarization of the emitted light occurs to 7 GPa. This behavior is opposite to the pressure-dependent reordering of the topmost valence band states in thin GaN/AlGa_N quantum wells which occurs from Γ_7 to Γ_9 states.

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1. Introduction

In the unstrained bulk GaN, the top valence subband is of Γ_9 symmetry, whereas in the bulk AlN, due to the negative value of the crystal field splitting energy, the sequence of subbands is inverted with the topmost subband having Γ_7 symmetry. This inversion results in different polarizations of the emitted light in the process of inter-band recombination and it may be obviously controlled in AlGa_N alloys by changing the Al concentration. The photon generated in the electron transition to the valence band Γ_9 state is emitted into so-called TE mode, polarized perpendicularly to the c axis, while the emission from the transition to the Γ_7 state occurs into the TM mode, polarized along the c axis. Consequently, the light extraction in the surface emitting devices based on [0001]-oriented AlGa_N/AlN structures becomes extremely difficult in the latter case. It has been demonstrated that the polarization switching from TE to TM mode resulting from the topmost valence band inversion in the emission from the AlGa_N epilayers grown on sapphire [0001] substrates with low temperature AlN buffer layers occurs at the critical concentration of Al equal to 0.25 [1]. It has been further shown that using the effect of quantum confinement in quantum wells (QWs) built with different material combinations employing AlN and AlGa_N as barrier and QW materials, respectively gives a possibility to modify the symmetry properties of the top of the valence band states in a QW structure pushing the critical content of Al for polarization switching to values as high as $x = 0.8$ [2] and thereby increasing substantially the wavelength range of efficient deep ultraviolet emitters. From these studies it was clear that the built-in strain originating from the lattice misfit between constituents plays a key role in determination of character of the topmost valence band state.

Recently, the influence of external hydrostatic pressure on the symmetry of the topmost valence band states has been investigated theoretically in [0001]-oriented GaN/

AlGa_N QWs lattice matched to GaN substrates [3]. It has been found for the structures with Al content in the barriers of 20% and the QW width of 1.5 nm that the reordering of the topmost valence band states from Γ_7 to Γ_9 occurs at pressure about 5 GPa [3]. It has been also pointed out that the excitonic effects may in general modify the simple relation between the band ordering and emitted light polarization switching. In the present work we extend this study to [0001]-oriented AlGa_N/AlN QWs emitting light in the deep ultraviolet range. These structures are the key components of deep-ultraviolet light emitting devices which find various applications, ranging from biological agent detection to next-generation data storage [2, 4].

2. Theoretical model

In order to investigate the effect of the external hydrostatic pressure on the valence band structure and optical transitions in nitride QWs, we have developed a model which fully takes into account (i) the influence of strain and the built-in electric fields on the conduction and valence band states in the QW and (ii) the excitonic effects which contribute significantly to the conditions for the reordering of corresponding optical transitions in emission and absorption spectra [3]. The model consists of two parts. First, the effective one-particle Hamiltonian for the QW including the influence of strain and the electric field due to the spontaneous polarization and piezoelectric effect is diagonalized in order to obtain one-electron spectra in the valence and conduction subbands. We consider full Rashba–Sheka–Pikus Hamiltonian for the valence band and anisotropic, parabolic Hamiltonian for the conduction band. In the second stage, the optical spectra are obtained by solving the Bethe–Salpeter exciton equation in the envelope function representation using Laguerre–Gauss orbitals basis set to describe the relative electron–hole motion [3]. The material parameters used in the calculations are taken from Table I in [3].

3. Results

The calculations have been performed for $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}$ QW structures with $x = 0.7$ and $x = 0.8$, respectively and the QW width of 1.5 nm. The structures were assumed to be lattice matched to AlN substrates. In Figs. 1 and 2 we show the between the energies of inter-band transitions to the two topmost valence band levels as a function of pressure for both QW structures for single particle (SP) levels and the difference in transition energies for excitonic transitions (X). First, we focus on the results for zero pressure. It follows from our calculations that for the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}$ QWs with $x = 0.7$, the topmost valence band is of Γ_9 symmetry while for the case of $x = 0.8$ it is of Γ_7 symmetry, quite well corresponding to the experimental results reported in [2]. From Fig. 1,

Fig. 1. Pressure dependence of the valence band levels energy difference $E_{\Gamma_9} - E_{\Gamma_7}$ (open squares) and difference of excitonic transition energies from the Γ_7 and Γ_9 subbands to the conduction band (full squares) in the 1.5 nm wide $\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}/\text{AlN}$ QW.

Fig. 2. As in Fig. 1, but for $\text{Al}_{0.8}\text{Ga}_{0.2}\text{N}/\text{AlN}$ QW.

it is clear that for the QW with $x = 0.7$ with increasing pressure, the symmetry of the topmost valence level is changing from Γ_9 state to Γ_7 at about 2.5 GPa while the polarization of the excitonic transition is changing at about 7 GPa. Let us note the non-linear dependence of the difference of energies of excitonic transitions on pressure. On the other hand, in the second structure (see Fig. 2), no change of the symmetry of the topmost valence level occurs although, similarly as in the previous case, the exciton effects decrease the transition energies difference between two different polarizations with respect to the single particle (SP) model.

4. Conclusions

We have studied theoretically the influence of the external hydrostatic pressure on the valence band structure in [0001]-oriented $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}$ QWs. The calculations performed using the multi-band $k \cdot p$ method with excitonic effects have revealed that for $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}$ QW with $x = 0.7$ and QW width of 1.5 nm, reordering of the topmost valence subbands having different symmetries occurs with increasing pressure. In these structures, at low pressure values the topmost valence level is of Γ_9 whereas it changes to the Γ_7 state for pressures about 2.5 GPa. The change of symmetry of the topmost valence subband results in switching of the polarization of the emitted light from the TE to TM mode. It turns out that the excitonic effects increase the critical value of pressure at which the polarization switching occurs to $p = 7$ GPa. This behavior is opposite to the pressure-dependent reordering of the topmost valence band states in thin GaN/AlGaIn QWs which occurs from Γ_7 to Γ_9 states. In both cases however, the excitonic effect introduces substantial modifications for the conditions for polarization switching.

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