EXCITON PROPERTIES OF NANOSCALE HETEROSTRUCRURES $Al_xGa_{1-x}N/GaN/Al_xGa_{1-x}N$

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Abstract. For the heterostructures Al_xGa_{1-x} N/GaN/Al_xGa_{1-x} N with different thicknesses of the GaN quantum wells and $Al_xGa_{1-x}N$ barriers, we use an exciton model, which includes the interaction of an electron and a hole with deformations of the crystal lattice and with built-in electrostatic fields. It is based on a 6-band hole Hamiltonian, as distinct from the variational approach. Exciton energy spectra and wave functions for the ground state and some excited states are found after a numerical diagonalization of the 6-band matrix hole Hamiltonian with an adaptive grid. The photoluminescence peak position, the exciton oscillator strengths and the exciton radiative lifetime have been investigated as a function of the thicknesses of quantum wells and barriers as well as of the concentration *x* of Al in the barrier .The developed theoretical approach has allowed us to interpret the position of the zero-phonon and one-phonon photoluminescence bands and to obtain the exciton radiative lifetime in a good agreement with experiment.

Key words: exciton, heterostructures, photoluminescence.

INTRODUCTION

Nitrides have been shown to be perspective materials for optoelectronics and electronics. A direct band gap, which can be changed from 1.5 eV till 6.0 eV depending on their composition, allows one to use these materials to fabricate photodiodes and lasers in a broad spectral range. Nitrides are wurtzite crystals with a strong spontaneous polarization causing the electrostatic fields with strength of several MV/cm [1] and high piezoelectric moduli (by one order of magnitude higher that those in CdS). Because of a large mismatch between adjacent crystal lattices in the AlGaN/GaN/AlGaN heterostructures, the deformations significantly influence the structure of the

energy bands and lead to the appearance of strong piezoelectric fields. In the structures with sufficiently wide GaN layers (> 5 nm), the potential of the built-in electrostatic field strongly bends the edges of the valence band and the conduction band. Due to this bending, a red shift of photoluminescence bands occurs.

The optical effects in the nitride-based heterostructures have been studied within one-band models of heavy and light holes, while the exciton states have been calculated variationally [2,3]. The size quantization leads to the intersubband mixing in the valence band. As a consequence, the excited exciton states cannot be found in the framework of a variational method. This was a motivation for us to analyze the problem using the 6-band hole Hamiltonian, as distinct from the variational approach.

RESULTS AND DISCUSSION

It is experimentally established that the GaN layers are unstrained, while the Al_xGa_{1-x} N layers at $x = 0.17$ [2] and $x = 0.24$ [3] are quasi-isomorphous, i.e., they have the same lattice constant as the GaN layers. Therefore in the GaN layers there exists only the spontaneous polarization, while both spontaneous and piezoelectric polarizations are in the $Al_xGa_{1-x}N$ layers. We found the electric fields in the layers taking into account that potentials on the outer surfaces of the structure are 0, and that Maxwellian boundary conditions are obeyed at all the interfaces. Therefore the fields in the wells and in the barriers are related to each other. We used the 6-band hole matrix Hamiltonian [4], which includes the spin-orbit interaction, the crystal-field splitting, the interaction with strain via the deformation potential, and the potential of the built-in electric field. The size-quantized energy spectrum and the wave functions for holes were obtained numerically, using the method of finite differences with an adaptive grid. The choice of the discretization increment of order 0.5 Å allowed us to find the hole energy levels with accuracy better than 1%.

The exciton Hamiltonian includes the electron and hole Hamiltonians, the energy of the Coulomb interaction between the electron and the hole as well as the self-action energy for charge carriers in the multi-layered structure. The exciton Hamiltonian is averaged using the size-quantized wave functions of the electron and hole, and then the Coulomb energy levels and wave functions, describing the intra-exciton in-plane motion, are found for each pair of the size-quantized electron and hole states.

The obtained size-quantized and Coulomb wave functions are further used as basis functions to represent the exciton wave function. The coefficients of this representation are obtained for 30 lowest exciton states.

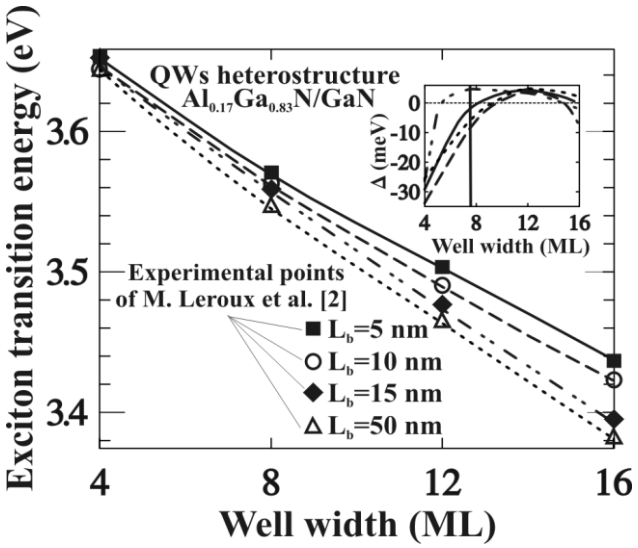

Fig. 1. Well-width dependence of the calculated exciton transition energies and experimental peak position [2].

In Fig. 1. the calculated results for the exciton transition energy are compared with the experimentally determined positions of the photoluminescence peaks as a function of the GaN quantum well width. In this figure are presented results for the $Al_{0.17}Ga_{0.83}N/GaN$ heterostructures including four GaN quantum wells: 4 monolayers (MLs), 8 MLs, 12 MLs, 16 MLs (1 ML = 0.259 nm) and the $Al_{0.17}Ga_{0.83}N$ barriers with different width [2]. The values of the deviation Δ of the variational results for the exciton transition energy of Ref. [2] from those calculated by us are shown in the insets to Fig. 1. It is worth noting that in Ref. [2] the values of the electric fields were deduced from the fit of the photoluminescence data for each of four quantum-well widths, while our calculation has been performed with one fitting parameter only.

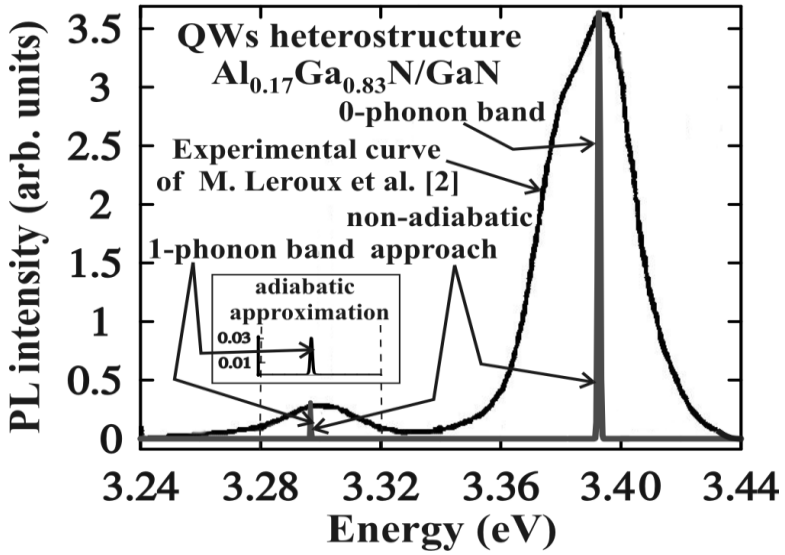

Fig. 2. Photoluminescence spectra of $Al_{0.17}Ga_{0.83}N/GaN$ heterostructure including four 16-ML quantum wells and 30-nm barriers.

In Fig. 2 we represent the experimentally observed [2] photoluminescence band together with its 1-phonon satellite and the results of our calculation of the positions of the 0-phonon and 1-phonon peaks. When calculating the exciton-phonon interaction, the wurtzite crystal structure in group-III nitrides was taken into account. As seen from Fig. 2, our theory compares well with experiment. The position and intensity of zero phonon peak obtained in the adiabatic approximation

are shown in the insets to Fig. 2. The adiabatic peak is ten times lower, than the peak calculated in the non-adiabatic approach [5]. Dependence of the radiative lifetime of exciton in ground state on the thickness of GaN well, calculated in this paper and obtained experimentally in Ref. [3] is shown in Fig. 3 for the $Al_{0.24}Ga_{0.76}N/GaN$ heterostructure. The developed theoretical approach has allowed us for the first time: (i) to describe the position of the photoluminescence bands in agreement with experiment [2,3], (ii) to explain the transition from the blue shift to the red shift in the photoluminescence spectra depending on the strength of the built-in electrostatic fields and the width of the well and barrier layers, (iii) to calculate the positions of the 0-phonon and 1-phonon peaks and their relative intensities in an excellent agreement of the experiment [2] and (iv) to estimate quantitatively the increase of the radiative relaxation time for the exciton with increasing the quantum well width.

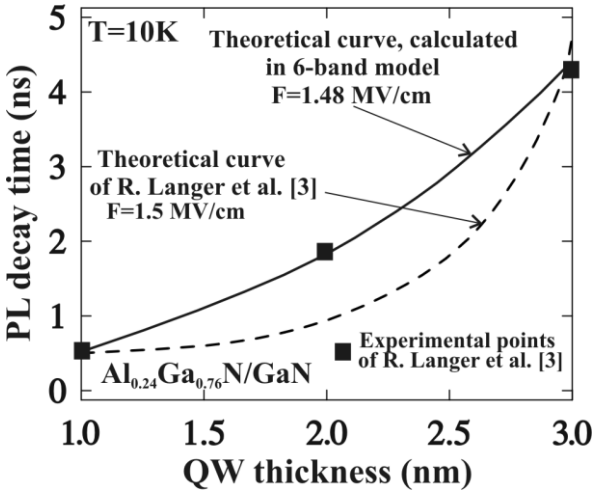

Fig. 3. PL decay time as a function of QW thickness for $Al_{0.24}Ga_{0.76}N/GaN$ heterostructures with 5-nm barriers.

This work was supported by FWO-V projects G.0274.01N, G.0435.03, the WOG WO.035.04N, GOA BOF UA 2000, IUAP (Belgium) and eiTT/COBRA Inter-University Research Institute (The Netherlands).

REFERENCES

[1] C. Adelman, E. Sarigiannidou, D. Jalabert, Y. Hori, J.-L. Rouviere, and B. Daudin, Appl. Phys. Lett. **82**, 4154 (2003).

[2] M. Leroux, N. Grandjean, J. Massies, B. Gill, P. Lefebvre and P. Bigenwald, Phys. Rev. B **60**, 1496 (1999).

[3] R. Langer, J. Simon, V. Ortiz, N. T. Pelekanos, A. Barski, R. Andre, and M. Godlewski, Appl. Phys. Lett., **74**, 3827 (1999).

[4] F. Mireles and S.E. Ulloa, Phys. Rev. B **60**, 13659 (1999).

[5] V. Fonoberov, E. P. Pokatilov, V. M. Fomin and J. T. Devreese, Phys. Rev. Lett, **92**, 127402 (2004).