XXXIX "Jaszowiec" International School and Conference on the Physics of Semiconductors, Krynica-Zdrój 2010

Pressure Dependence of Exciton Binding Energy in $GaN/Al_xGa_{1-x}N$ Quantum Wells

W. Bardyszewski[a], S.P. Łepkowski[b] and H. Teisseyre[b,c]

[a]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warszawa, Poland

[b]Institute of High Pressure Physics, "Unipress", Polish Academy of Sciences
Sokołowska 29/37, 01-142 Warszawa, Poland

[c]Institute of Physics, Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warszawa, Poland

We present a theoretical study of excitons in $GaN/Al_xGa_{1-x}N$ wurtzite (0001) quantum wells subjected to hydrostatic pressure. Our results show that the combined effect of pressure induced changes in band structure and piezoelectric field leads to reduction of the exciton binding energy. This subtle effect is described quite accurately by our multiband model of excitons in quantum wells.

PACS: 78.40.Fy, 78.20.Bh, 78.30.Fs

1. Introduction

Anomalous pressure dependence of the optical properties of nitride quantum structures attracted a lot of attention in recent years. It has been demonstrated that the strong piezoelectric fields existing in wurtzite heterostructures grown in the (0001) direction reduce substantially the pressure coefficient of the light emission in the nitride based quantum wells as compared to the pressure coefficient of the energy gap in unstrained bulk materials [1–3]. This effect was attributed mainly to the pressure induced enhancement of the piezoelectric field. These studies based on the band to band photoluminescence measurements usually ignored the pressure effect on the exciton binding energy assuming that its contribution to the overall effect is small [2, 3]. Recent theoretical analysis [4] employing a simple two band variational technique indicated that the exciton binding energy in $GaN/Al_xGa_{1-x}N$ quantum wells with barrier composition $x = 0.3$ and well thickness equal to 30 Å indeed increases only slightly with pressure at the rate of about 0.1 meV per 1 GPa. In order to verify this result we applied a comprehensive model of excitonic spectra in wurtzite type quantum wells taking into account the complicated band structure in such systems.

2. Model

We find the excitonic spectra using the Kubo formalism for the dielectric function. To this end we solve the Bethe–Salpeter equation using the single particle basis states constructed from products of envelope functions in the quantum well growth direction and Landau level orbitals describing the relative electron–hole motion in the quantum well plane. The envelope functions are obtained using a finite element method while the Landau level orbitals are evaluated for a fictitious magnetic field B_0 which can be adjusted in order to increase the accuracy of calculations [5]. The pressure induced changes in band structure and the piezoelectric field are incorporated in the shape of the envelope wave functions. We have also taken into account the pressure dependence of the dielectric constant. Consequently the influence of pressure on effective electron–hole Coulomb interaction and the in-plane kinetic energy in the quantum well is fully taken account. In addition, we incorporate the effects of mirror symmetry breaking caused by the strong electric field as well as the electron–hole exchange. The exciton binding energies are obtained from the analysis of the theoretical absorption spectra. Although in our calculations we did not have to resort to the so-called quasi-cubic approximation, there is still a big uncertainty regarding the values of the valence band parameters of bulk materials. Of particular importance are the so-called crystal field and spin–orbit splitting parameters. The experimental determination of their values is usually biased by the possible built-in strain resulting from the epitaxial growth. In our calculation we have used well established set of parameters proposed in [6] even though recently a big modification of their values was suggested in [7]. Due to existing discrepancies and lack of information regarding the pressure dependence of the bulk valence band parameters in GaN in AlN we have neglected their pressure dependence altogether.

3. Results and discussion

Hydrostatic pressure applied to wurtzite $GaN/Al_xGa_{1-x}N$ structures modifies electronic states, in particular by increasing the band offset and increasing the electric field [3]. This last phenomenon is related to nonlinear piezoelectric effect. Therefore, we expect a com-

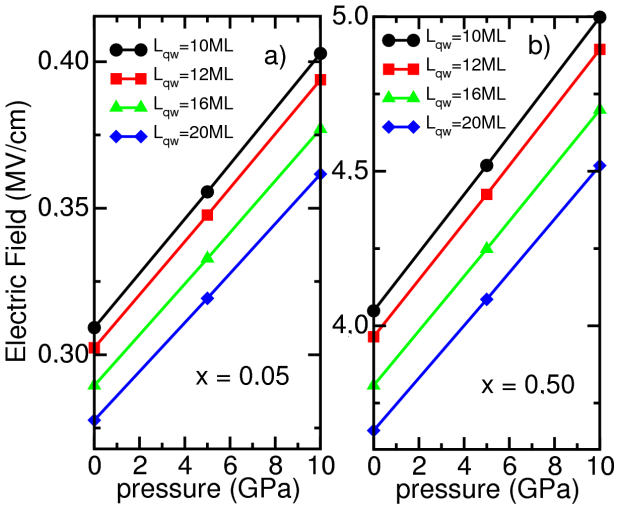

Fig. 1. Electric field in $GaN/Al_xGa_{1-x}N$ quantum wells for various well widths and barrier composition: (a) for $x = 0.05$ and (b) for $x = 0.50$.

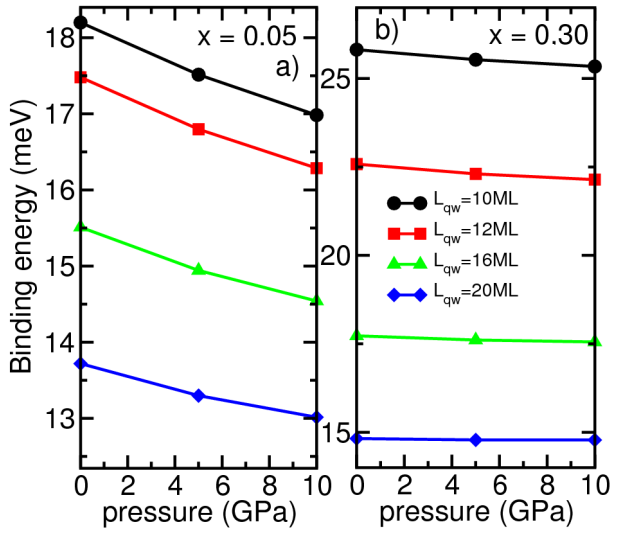

Fig. 2. Exciton binding energy shift with pressure in $GaN/Al_xGa_{1-x}N$ quantum wells for various well widths and barrier composition: (a) for $x = 0.05$ and (b) for $x = 0.30$.

petition between two effects on the binding energy of excitons under pressure: (i) reduction of the Coulomb interaction due to the spacial separation of electron and hole wave functions in growth direction caused by the pressure induced increase of the piezoelectric field and (ii) larger band-offset and stronger confinement of electrons and holes in the growth direction. The first effect would lead to reduction of the binding energy while the latter would result in the bigger binding energy of excitons. There is, in fact, also a third mechanism related to the fact that the exciton binding energy in bulk AlN is much larger than in GaN due to the larger valence band

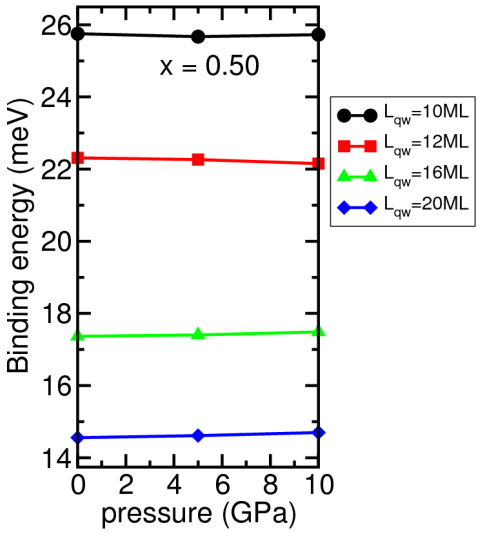

Fig. 3. Exciton binding energy shift with pressure in $GaN/Al_xGa_{1-x}N$ quantum wells for various well widths and for the barrier composition $x = 0.50$.

effective mass in AlN. The enhanced penetration of the $Al_xGa_{1-x}N$ barrier by the valence band wave function at high electric field (high concentration of Al in the barrier) may therefore lead to the increased exciton binding energy. There are then two mechanisms associated with the presence of piezoelectric field as far as the exciton binding energy is concerned — the reduction of the potential energy due to the separation of the electron and hole wave functions and reduction of the kinetic energy of the hole due to the increased effective mass for the in-plane direction. Thus we may expect different behavior of the exciton binding energy depending on the prevailing mechanism. Calculations were performed for a range of quantum well widths equal to 10, 12, and 16 monolayers and for Al content in the barrier equal to 5, 30 and 50 percent. The piezoelectric field dependence on the hydrostatic pressure for different quantum well widths is shown in Fig. 1. The field is relatively weak for barriers with low Al concentration ($x = 0.05$) and may reach values as high as 5 MV/cm for $x = 0.5$. In this latter case the pressure induced change of the electric field takes the value of almost 1 MV/cm for the pressure $p = 10$ GPa.

The character of the binding energies dependence on pressure varies with the quantum well width and barrier composition, as illustrated in Fig. 2. The change of the binding energy with pressure is most prominent for narrow quantum wells. As shown in Figs. 2a and b, the exciton binding energy decreases with pressure for low concentration of Al in the barrier, $x < 0.5$, while it is almost pressure independent or even tends to slightly increase for wider wells at $x = 0.5$ as illustrated in Fig. 3. This is probably caused by the fact that at high electric field, the effect of increased effective mass compensates the reduction of the Coulomb attraction between the electron and the hole. Our results, although in principle confirming

the weak dependence of the exciton binding energy on pressure show opposite trends as compared to the simple model used in [4]. For lower concentration of Al in the barrier we predict a slight reduction of the binding energy with pressure while for higher contents, the binding energy is almost pressure insensitive or increases very slightly at very high electric field, while a simple single band model of excitons employed in [4] predicts increase of the exciton binding energy with pressure.

Acknowledgments

This work was supported by the Polish State Committee for Scientific Research, project No. NN202 010134.

References

[1] S.P. Łepkowski, H. Teysseyre, T. Suski, P. Perlin, N. Grandjean, J. Massies, *Appl. Phys. Lett.* **79**, 1483 (2001).

[2] G. Vaschenko, D. Patel, C.S. Menoni, N.F. Gardner, J. Sunb, W. Gotz, C.B. Tome, B. Clausen, *Phys. Rev. B* **64**, 241308 (2001).

[3] S.P. Łepkowski, J.A. Majewski, G. Jurczak, *Phys. Rev. B* **72**, 245201 (2005).

[4] S.H. Ha, S.L. Ban, *J. Phys., Condens. Matter* **20**, 085218 (2008).

[5] M. Sobol, W. Bardyszewski, *Phys. Rev. B* **73**, 075208 (2006).

[6] S.-H. Park, S.L. Chuang, *J. Appl. Phys.* **87**, 353 (2000).

[7] B. Gil, *Phys. Rev. B* **81**, 205201 (2010).