Proceedings of the 43rd "Jaszowiec", International School and Conference on the Physics of Semiconductors, Wisła 2014

Polarization-Induced Band Inversion in In-Rich InGaN/GaN Quantum Wells

S.P. Łepkowski[a], W. Bardyszewski[b] and D. Rodak[b]

[a]Institute of High Pressure Physics — Unipress, Polish Academy of Sciences, Sokołowska 29, 01-142 Warszawa, Poland

[b]Faculty of Physics, University of Warsaw, L. Pasteura 5, 02-093 Warszawa, Poland

We theoretically study the polarization-induced band inversion phenomenon in c-plane In-rich InGaN/GaN quantum wells. Our calculations performed using the $k \cdot p$ method with the 8×8 Rashba–Sheka–Pikus Hamiltonian for the structures with the indium content between 90% and 100% show that the reordering of the conduction and valence bands occurs for the quantum well widths below the theoretical values of critical thickness for InGaN layers pseudomorphically grown on GaN substrates.

DOI: 10.12693/APhysPolA.126.1154

PACS: 73.21.Fg, 73.22.Dj

1. Introduction

InN and In-rich InGaN alloys have been attracting attention as important nitride semiconductors which allow to move the spectrum of light emission from the blue-UV region towards the green, red, and infrared wavelengths. This possibility is associated with the narrow band gap of InN equal approximately to 0.7 eV. Growing high-quality InGaN layers with high In content on GaN substrates is difficult due to the large lattice mismatch between InN and GaN. To overcome this problem ultrathin InN/GaN quantum wells (QWs) and superlattices have been considered [1]. It has been shown theoretically by means of the *ab initio* calculations that in these structures grown along c crystalline axis, the energy gap at the Γ point of the Brillouin zone changes dramatically with the QW width from about 2 eV for 1 monolayer (ML) of InN to 0 eV, with inverted order of the conduction and valence band states, for 3–4 MLs of InN [2]. This effect is associated with the presence of the built-in electric fields originating from the spontaneous and piezoelectric polarizations. The magnitude of the built-in electric field in InN/GaN QWs can reach 12–13 MV/cm which leads to a substantial potential drop over the InN region even for a few MLs thin QWs. The band inversion predicted for InN/GaN QWs with 4 MLs of InN was used to suggest the possibility of existence of a topological insulator state in these structures [2].

In this work, we extend the theoretical study of the polarization-induced band inversion phenomenon to c-plane In-rich InGaN/GaN QWs. Our calculations performed for the structures with the indium content between 90% and 100% show that the reordering of the conduction and valence bands occurs for the QW thicknesses below the theoretical values of critical thickness for pseudomorphic growth of $In_xGa_{1-x}N$/GaN QWs.

2. Theoretical model

In order to describe the electronic band structure of indium rich InGaN/GaN QWs we use the $k \cdot p$ method with the 8×8 Rashba–Sheka–Pikus Hamiltonian, which takes into account the coupling between the conduction states of Γ_7 symmetry and valence band states transforming according to the Γ_9 (heavy holes) and Γ_7 (light and spin–orbit split-off holes) symmetries. The band structure parameters for this Hamiltonian have been obtained by interpolating the literature data for GaN and InN from Refs. [2] and [3]. In order to take into account the broken translational symmetry in the direction perpendicular to the QW plane, the z-component of momentum in the Hamiltonian is replaced by the $-\mathrm{i}\hbar\frac{\partial}{\partial z}$ operator. Resulting system of 8 differential equations is solved using the finite element method. Strain and the built-in electric field entering the Hamiltonian are determined using the nonlinear theory of elasticity and piezoelectricity including contributions arising from the second-order piezoelectric constants and the third-order elastic constants [4].

3. Results

The band structure calculations have been performed for InGaN/GaN QWs lattice matched to GaN substrate with the In content equal to 100%, 95%, and 90%. The QW width has been changed from 1.3 nm to 2 nm, while the barrier thickness was kept at 40 nm.

In Fig. 1a and b, we show the electronic band structures in the vicinity of the Γ point for two InN/GaN QW structures with the QW width equal to 1.4 and 1.6 nm, respectively. Situation presented in Fig. 1a corresponds to the normal ordering of bands with the Γ_7 conduction band states (grey line) lying above the valence bands states (black lines), whereas in Fig. 1b the ordering of bands is reversed for small values of the in-plane wave vector $\boldsymbol{k}_{\parallel}$. It is worth noting that for large values of $\boldsymbol{k}_{\parallel}$, the ordering of bands is restored to the normal band structure.

In Fig. 2 we present the dependence of the band energy difference at the Γ point between the Γ_7 conduction band state and the Γ_9 valence band state on the QW width for InN/GaN, $In_{0.95}Ga_{0.05}N$/GaN and $In_{0.9}Ga_{0.1}N$/GaN

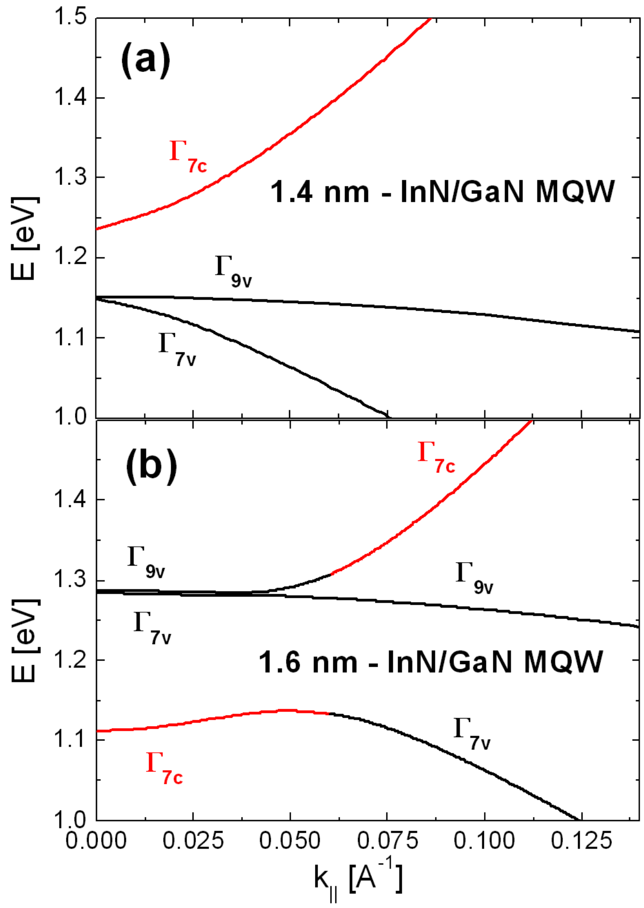

Fig. 1. Band structure of InN/GaN QWs in the vicinity of the band gap for the QW width of (a) 1.4 nm and (b) 1.6 nm. The grey (red on-line) color reflects the states with the dominant contribution from the conduction band *s*-type states, while the black color corresponds to the dominant valence band *p*-states.

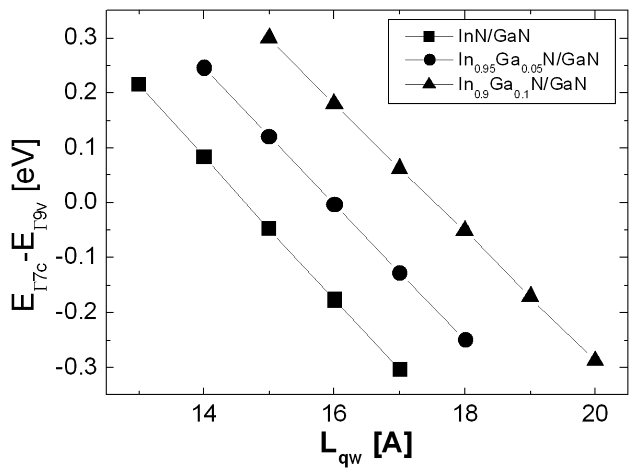

Fig. 2. The dependence of the difference between the Γ_7 conduction band state and the Γ_9 valence band state on the QW width in InN/GaN, $In_{0.95}Ga_{0.05}N$/GaN, and $In_{0.9}Ga_{0.1}N$/GaN QW structures.

QW structures. It can be observed that for InN/GaN QWs, the transition from the normal to inverted band structure occurs at the QW thickness equal to 1.5 nm which corresponds very well to the results presented in Ref. [2]. Increasing Ga content in the QW region shifts the critical QW width corresponding to the band inversion to 1.6 nm and 1.8 nm for $In_{0.95}Ga_{0.05}N$/GaN and $In_{0.9}Ga_{0.1}N$/GaN, respectively. The dependence of the energy gap on the QW width has almost the same slope in all three cases.

4. Conclusions

We have analyzed the polarization-induced band inversion effect in In-rich, fully strained $In_xGa_{1-x}N$/GaN QWs. Our calculations performed for the structures with the indium content between 90% and 100% have shown that the reordering of bands occurs for the QW widths below the theoretical values of critical thickness for pseudomorphic growth of $In_xGa_{1-x}N$/GaN QWs [2]. Therefore, obtaining fully strained indium rich $In_xGa_{1-x}N$/GaN QWs with inverted band structures seems to be experimentally available.

Acknowledgments

S.Ł. thanks K. Sakowski for useful discussion concerning the finite element method. This work was supported by the Polish National Science Center, Project No. 2012/07/B/ST3/03174.

References

[1] M.S. Miao, Q.M. Yan, C.G. Van de Walle, *Appl. Phys. Lett.* **102**, 102103 (2013).

[2] M.S. Miao, Q.M. Yan, C.G. Van de Walle, W.K. Lou, L.L. Li, K. Chang, *Phys. Rev. Lett.* **109**, 186803 (2012).

[3] P. Rinke, M. Winkelnkemper, A. Qteish, D. Bimberg, J. Neugebauer, M. Scheffler, *Phys. Rev. B* **77**, 075202 (2008).

[4] J. Pal, G. Tse, V. Haxha, M.A. Migliorato, S. Tomic, *Phys. Rev. B* **84**, 085211 (2011).