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

Sławomir P. Łepkowski[1], Witold Bardyszewski[2], and Daniel Rodak[2]

[1]*Institute of High Pressure Physics - Unipress, Polish Academy of Sciences, ul. Sokołowska 29, 01-142 Warsaw, Poland*
[2]*Faculty of Physics, University of Warsaw, ul. Hoża 69, 00-681 Warszawa, Poland*

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 ultra-thin InN/GaN quantum wells (QWs) and superlattices have been investigated [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 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 4MLs 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 grown on GaN substrates. Our calculations are performed in the framework of the k·p method with the 8x8 Rashba-Sheka-Pikus Hamiltonian which takes into account the coupling between the conduction and valence band states. Strain and the built-in electric field 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 [3, 4].

The band structure calculations have been performed for InGaN/GaN QWs with the In content equal to 100%, 95%, and 90%. The well thickness was changed from 1.3 nm to 2 nm, while the barrier thickness was kept at 40 nm. The obtained results show that for InN/GaN QW, 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 structures, respectively. The dependence of the energy gap on the QW width has the same slope in all three cases.

This work was supported by the Polish National Science Center, Project No. 2012/07/B/ST3/03174.

[1] M. S. Miao, Q. M. Yan, and C. G. Van de Walle, *Appl. Phys. Lett*. **102**, 102103 (2013).
[2] M. S. Miao, Q. M. Yan, and C. G. Van de Walle, W. K. Lou, L. L. Li, and K. Chang, *Phys. Rev. Lett*. **109**, 186803 (2012).
[3] J. Pal, G. Tse, V. Haxha, M.A. Migliorato, and S. Tomic, *Phys. Rev. B* **84**, 085211 (2011).
[4] S. P. Łepkowski, (private communication).