Pressure dependence of GaN/AlN quantum wells properties by density functional theory with half occupation technique correction

Pawel Strak[1], Agata Kaminska[2], Pawel Kempisty[1], Konrad Sakowski[1], and Stanislaw Krukowski[1,3]

[1]*Institute of High Pressure Physics, Polish Academy of Sciences, Sokolowska 29/37, 01-142 Warsaw, Poland*

[2]*Institute of Physics Polish Academy of Sciences, Al. Lotnikw 32/46, 01-142 Warsaw, Poland*

[3]*Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Pawinskiego 5a, 02-106 Warsaw, Poland*

In the following we presented detailed analysis of physical properties of GaN/AlN MQWs system with respect to wells and barriers width, and with respect to different strain stress conditions including hydrostatic pressure case. The influence of strain, hydrostatic, tetragonal and uniaxial was analyzed. It was shown that tetragonal strain related to lattice mismatch is responsible for the drastic decrease of pressure coefficients of photoluminescence energy observed for polar MQWs. Applied pressure increases the electric field in the well and the barrier considerably. It contribute to the decrease of pressure coefficient observed experimentally in polar wells. At the heterointerface between AlN and GaN the potential drops emerges such that the GaN part has the potential about 2 V higher than AlN. The potential jump is very abrupt, occurs within single unit cell. The potential jumps weakly depend on the tetragonal strain and also on the applied pressure. The data indicate that the dipole layer is not susceptible to the mechanical strain. Finally, the changes of the bandgap, induced by the effect of tetragonal and unixial strains as well as the pressure, were determined. It was shown that the tetragonal strain is highly different in case of stretching and compressing. The stretching leads to a linear decrease of the bandgap, while for a tetragonal compression the decrease is highly nonlinear. The value of bandgap energy change is 0.5 eV for AlN stretched to GaN. For GaN compressed to AlN, the change is highly nonlinear and is relatively small compared to linear change, about 3%. The effect of uniaxial strain is highly nonlinear for AlN, both free and tetragonally strained to GaN. For GaN, the situation is different. The bandgap changes in a nonlinear way for free GaN while the tetragonally-strained GaN behaves linearly for a wide range of deformations. The analysis of the thin layers fully strained to a thick substrate was made. It was shown that in the linear regime, the substrates influence changes the effect induced by pressure due to a different stiffness of the substrate and the layer. Using the mechanical analysis a pressure-related change of the bandgap and the polarization was obtained. It was shown that the bandgap change due to quantum overlap has a relatively small contribution whilst the piezo effects have a dominant contribution to the decrease of pressure coefficient of the PL energy. The decrease of the coefficient is caused by the tetragonal strain which may lead to a change of sign of the coefficients for wider wells and barriers.