phys. stat. sol. (c) **2**, No. 3, 972–975 (2005) / **DOI** 10.1002/pssc.200460604

Modeling of elastic, piezoelectric and optical properties of vertically correlated GaN/AlN quantum dots

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Received 8 September 2004, revised 20 September 2004, accepted 22 September 2004
Published online 18 February 2005

PACS 68.35.Gy, 68.65.Hb, 78.67.Hc

We theoretically investigate elastic, piezoelectric and optical properties of wurtzite GaN/AlN quantum dots, having hexagonal pyramid-shape, stacked in a multilayer. We show that the strain existing in quantum dots and barriers depends significantly on the distance between the dots i.e. on the width of AlN barriers. Drop of the electrostatic potential in the quantum dot region slightly increases with increasing of the barrier width. This increase is however much smaller for QDs than for superlattice of quantum wells. Consequently, band-to-band transition energies in the vertically correlated quantum dots show rather weak dependence on the width of AlN barriers.

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1 Introduction For the last few years, nitride quantum dots (QDs) have attracted considerable attention due to their promising applications. On the one hand, in short-wavelenght optoelectronics, self-organized GaN/AlN or InGaN/GaN QDs are considered as new candidates for the active region in blue or UV light emitters [1]. One expects that the three dimensional carrier confinement present in nitride QDs can increase the optical material gain and decrease the non-radiative recombination in comparison with conventionally used nitride quantum wells. On the other hand, strong built-in electric fields present in nitride QDs, due to spontaneous and piezoelectric polarizations, make these structures attractive for quantum information processing or spintronics [2, 3]. This is mainly due to strong and intrinsic exciton-exciton coupling possible in these structures.

Both mentioned fields of potential applications of nitride QDs are connected with vertical stacking of QDs in the multilayer. Recently, there have been a few reports on successful growth of vertically correlated wurtzite GaN/AlN QDs stacked in multilayers [4–6]. The strong vertical ordering, along the (0001) direction, observed in the multilayers of wurtzite GaN/AlN QDs is attributed to a local lattice distortion enhancement localized directly above the previously buried QD [7].

Theoretical study of optical properties of wurtzite GaN/AlN QDs have already been performed by several groups. In Ref. [8], a semi-analytic approach based on the plane wave expansion method was used to calculate strain distribution, electrostatic potential and electronic states in GaN/AlN QDs. Comprehensive tight-binding calculations of electronic structure in InGaN/GaN QDs were presented in Ref. [9]. Excitonic properties of GaN/AlN QDs together with finite difference/finite element modeling of strain and electrostatic potential were reported in Ref. [10]. However, all the above papers focus on the properties of a single QD, rather than on the correlation between dots stacked in multilayer. This remark

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applies also to Ref. [8], although the plane wave expansion method used in that paper is naturally useful to deal with periodic multilayers of QDs.

In this paper, we investigate elastic, piezoelectric and optical properties of wurtzite GaN/AlN QDs, having hexagonal pyramid-shape, stacked in the multilayer. We show how strain, electrostatic potential and energy of band-to-band transition depend on the height of the QDs, L_d, and the width of AlN barrier, L_{br}.

2 Theoretical model We have developed a numerical model, based fully on the finite element method, which accurately determines strain distribution, piezoelectric fields and electronic states in wurtzite QDs of arbitrary shape. The calculations start from solving the boundary-value problem for elasticity using the nonlinear anisotropic hyperelasticity based upon the general strain measure [11]. Calculations of elastic relaxation phenomena in the heterostructure allow us to determine the strain field, which is used to calculate piezoelectric polarization. The piezoelectric fields caused by spontaneous and piezoelectric polarizations are considered. Distribution of the electrostatic potential is calculated by solving the Poisson equation while the electronic states are obtained by using 8x8 k·p hamiltonian of the wurtzite crystal.

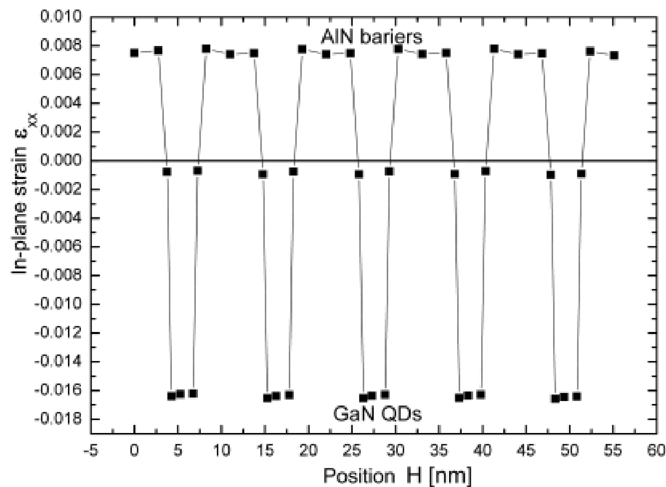

Fig. 1 In-plane strain ε_{xx} for the stack of five QDs (L_d=3 nm and L_{br} = 7.5 nm) as a function of position in a structure (along axis (0001)).

Our calculations are divided into two steps. First, we calculate the stress and strain distribution, the piezoelectric fields and the electrostatic potential for the sequence of five GaN/AlN QDs placed one on another in the direction of growth. This allows us to examine the correlations of strain and piezoelectric fields between QDs in the multilayer. Second, for the central QD, we calculate electronic states using boundary conditions obtained from previous step. In this way, we are able to deduce how the vertical correlation of QDs affects their optical properties. In this procedure we neglect quantum mechanical correlations between the dots. For this reason the model is valid for the case when the distance between the dots is high enough to prevent effective tunneling of carriers. This is however typical experimental situation since the AlN barriers between the dots are usually higher than 5 nm [4-6].

3 Results and discussion We have performed calculations for several structures assuming QDs height L_d= 2,3,4 nm and distance between dots L_{br}= 5-10 nm. In Fig. 1, we present the distribution of a in-plane strain, ε_{xx}, for the stack of five QDs with L_d=3 nm and L_{br} = 7.5 nm. The magnitude of the strain ε_{xx} has been taken along axis (0001), parallel to the direction of growth and located in the center of QDs. One can see that ε_{xx} is negative and practically constant inside QDs and positive and also nearly constant inside AlN barriers.

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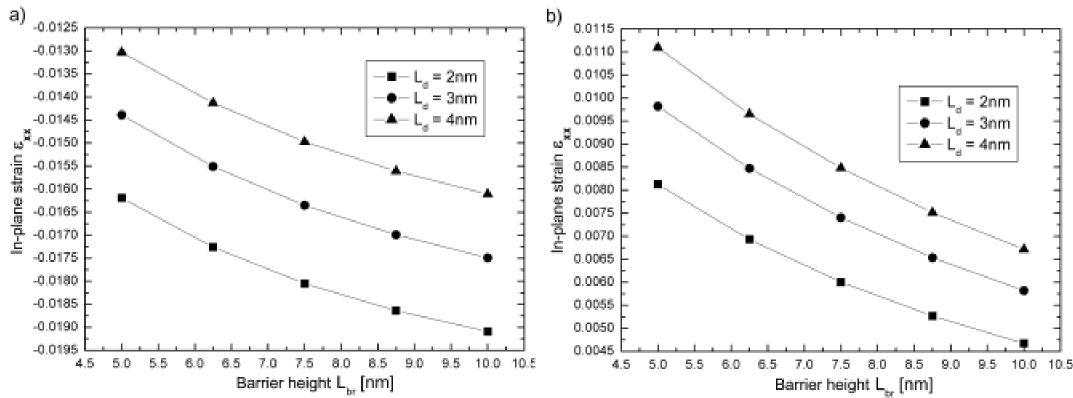

Fig. 2 In-plane strain, ε_{xx}, in GaN QDs (a) and AlN barriers (b) as a function of L_d and L_{br}. Solid lines are added to guide the eye.

In Fig. 2, we show in-plane strain, ε_{xx}, for the QD region (a) and the AlN barriers (b) calculated for structures with different L_d and L_{br}. The compressive strain in QDs increases with increasing L_{br}, while in the barriers, tensile strain decreases with increasing L_{br}. This effect can be explained by a simple argument that residual stresses in a layer of a multilayer stack decrease with increasing its thickness to preserve equilibrium. Simultaneously, for neighboring layers stresses increase.

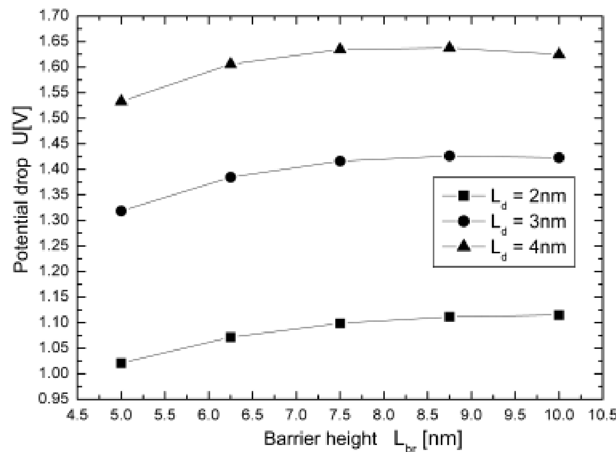

Fig. 3 Dependence of potential drop U as a function of L_d and L_{br}. Solid lines are added to guide the eye.

The strain field generates piezoelectric polarization which together with spontaneous polarization introduce bending of conduction and valence band states due to Quantum Confine Stark Effect (QCSE). The magnitude of QCSE is proportional to the drop of electrostatic potential in the region of the QD i.e. the difference between the values of potential at the top and at the bottom surfaces of the QD. In Fig. 3, we present the dependence of electrostatic potential drop U, on L_d and L_{br}. We observe slight increase of U with increasing L_{br}. The increase of U is much weaker than for the superlattice of quantum wells calculated using analytic model taken from Ref. [12]. This small dependence of U on L_{br} for QDs results in small variation of band-to-band transition energy with L_{br}, what is shown in Fig. 4. This is in contrast to the case of quantum wells when significant changes in energy emission were observed for different thickness of barriers [13]. In Fig. 4, we show additionally the measured values of energy emission for the series of vertically correlated QDs structures width different height of QDs, taken from Ref. [4]. The agreement of experimental data with our results is quite good.

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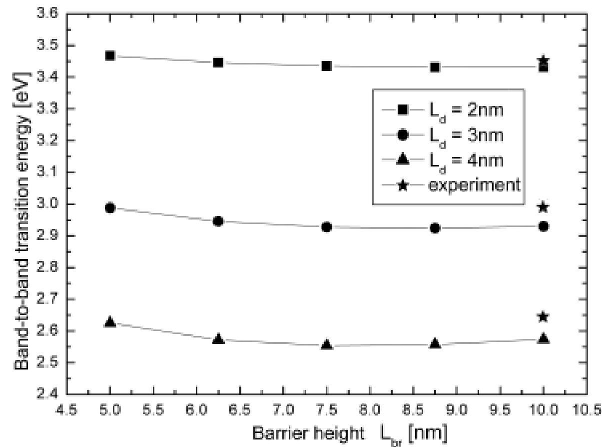

Fig. 4 Band-to-band transition energies for different L_d and L_{br}. Experimental points are taken from Ref. [4]. Solid lines are added to guide an eye.

4 Conclusions We have investigated elastic, piezoelectric and optical properties of wurtzite GaN/AlN QDs, having hexagonal pyramid-shape, stacked in the multilayer. We have shown that the strain the QDs and barriers depends significantly on the distance between the dots i.e. on the width of AlN barriers. Drop of the electrostatic potential in the QD region slightly increases with the width of barriers. This increase is however much smaller for QDs than for superlattice of quantum well. The band-to-band transition energies in the vertically correlated QDs show rather weak dependence on the width of AlN barriers.

Acknowledgements We would like to thank Prof. S. Krukowski from Unipress, High Pressure Research Center, Polish Academy of Sciences for very helpful discussions. This work has been supported by the Polish State Committee for Scientific Research, Project No. 4T11F 008 25 and ICMUW (computing facilities).

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