Journal of the Korean Physical Society, Vol. 57, No. 5, November 2010, pp. 1308∼1311 Brief Reports

Polarization Potentials in InGaN/GaN Semiconductor Quantum Dots

Seoung-Hwan Park and Woo-Pyo Hong*
Department of Electronics Engineering, Catholic University of Daegu, Kyeongsan 712-702, Republic of Korea

(Received 5 August 2010)

The polarization potentials as functions of the wetting layer thickness and the In composition in InGaN/GaN semiconductor quantum dots are investigated using the theory of continuum elasticity based on a three-dimensional finite element method. The strain-induced potential is found to increase rapidly with increasing In composition. The potential is almost entirely contributed by the strain-induced piezoelectric polarization, irrespective of the In composition. The total potential at the boundary between the quantum dot and the barrier regions gradually increases with increasing wetting layer thickness. Hence, the optical properties are expected to depend highly on the wetting layer thickness.

PACS numbers: 42.55.Px, 42.60.-v, 71.22.+i, 72.80.Ey
Keywords: InGaN, GaN, Quantum Dot, Strain, Piezoelectric, Polarization Potential
DOI: 10.3938/jkps.57.1308

I. INTRODUCTION

Recently, wide band-gap wurtzite (WZ) semiconductors have attracted much attention due to their potential applications for optoelectronic devices in the blue and the ultraviolet (UV) regions. The (0001)-oriented WZ structure leads to strong internal fields of the order of MV/cm in quantum wells (QWs) and heterostructures [1,2]. The internal fields become larger when the In composition or the well width is increased in InGaN/GaN QW structures, which leads to a larger spatial separation between the electron and the hole wavefunctions. Along with the strong interest in the influence of the In composition and the well width on the electronic and the optical properties of InGaN/GaN QW structures, there has been increasing interest in nitride-based quantum dot (QD) structures [3]. There are two contributions to the internal potentials in these systems; the first, referred to as the spontaneous potential, arises due to the difference between the QD and matrix materials; the second, referred to as the strain-induced piezoelectric potential, arises due to strain-induced lattice distortions. Thus, detailed knowledge of the internal potentials and the strain fields in and around the QDs can serve as a useful tool to understand their electronic and optical properties. Despite their importance, however, many fundamental characteristics of the polarization potentials in InGaN/GaN semiconductor QDs are still not well understood.

In this research, we investigated the polarization potentials as functions of the wetting layer thickness and the In composition in InGaN/GaN semiconductor QDs. Experimental studies indicate that real nitride quantum dots have a truncated hexagonal pyramid shape [4]. However, it was shown that the potential within a truncated hexagonal pyramid QD could be well approximated by that of a truncated-cone QD of the same volume and shape [3]. Here, we assumed a truncated-cone QD instead of a truncated-hexagonal- pyramid QD in the following analysis.

II. THEORETICAL MODEL

The piezoelectric coupling in III-V compound semiconductors is due to the ionic bonding between Type A (cation) and Type B (anion) atoms. Displacements of crystal atoms from their equilibrium positions give rise to local atomic dipoles and an electric field. This electric field subsequently induces a force opposing the displacement. The electric interaction of the ionic crystal, therefore, couples the elastic strain to the internal electric field. The vectors of the stress σ and the electric flux D are related to the strain ϵ and the electric field E vectors as [5]

$$\begin{aligned} \sigma_{ij} &= C_{ijlm}\epsilon_{ij} - e_{kji}E_k, \\ D_i &= e_{ijk}\epsilon_{jk} + \epsilon_0\epsilon_r E_j + P_{sp}, \end{aligned} \quad (1)$$

where C_{ijlm}, e_{kji}, and ϵ_r are the elastic moduli, piezoelectric coefficients, and relative dielectric constants, respectively. The elastic strain and piezoelectric potential were calculated using the theory of continuum elasticity and a finite-element method (FEM) [6–8]. Here, P_{sp}

*E-mail: wphong@cu.ac.kr

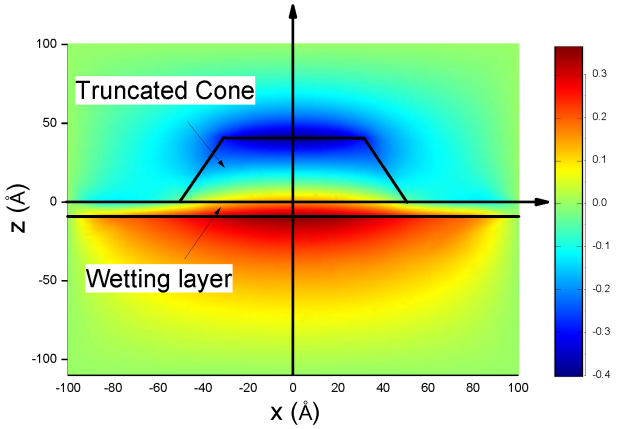

Fig. 1. (Color online) Plot for the potential in the r-z plane of a InGaN/GaN truncated cone QD. The height of the QD and the diameters of the circles at the bottom and the top are fixed to be 4.0 nm, 5.0 nm, and 3.0 nm, respectively.

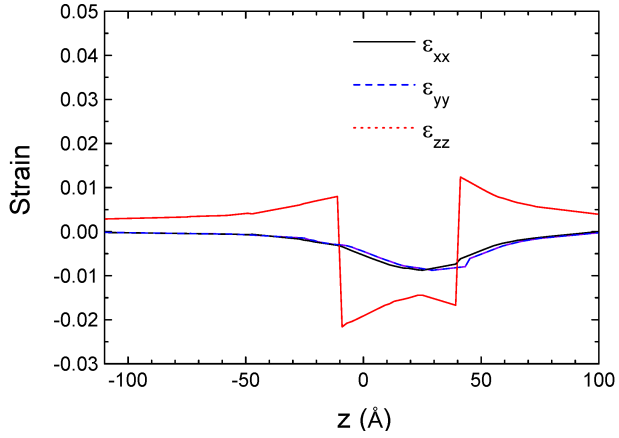

Fig. 2. (Color online) Strain field along the z-axis of a InGaN/GaN truncated- cone QD with a wetting layer thickness of 1.0 nm.

corresponds to the spontaneous polarization. Usually, the polarizations in WZ semiconductors arises from two sources; one is the strain-induced piezoeletric polarization, and the other is spontaneous polarization. The strain-induced piezoelectric polarization is given by

$$P_i = e_{ijk}\epsilon_{jk}. \tag{2}$$

The spontaneous polarization arises because the dimensions and the atom sites of a III-N unit cell differ slightly from those of an ideal hexagonal crystal. This deviation introduces spontaneous polarization along the c-axis or the z-direction. Symmetry considerations allow 27 constants for e_{ijk} to be reduced to just three independent components for the wurtzite nitrides (GaN, AlN, InN), which, for convenience, are renamed $e_{15} = e_{113} = e_{223}$, $e_{31} = e_{311} = e_{322}$, and $e_{33} = e_{333}$. Thus, the total polarization on the right-hand side of Eq. (1) is given by

$$\mathbf{P} = \begin{pmatrix} 2e_{15}\epsilon_{13} \\ 2e_{15}\epsilon_{23} \\ e_{31}(\epsilon_{11}+\epsilon_{22}) + e_{33}\epsilon_{33} + P_{sp} \end{pmatrix}. \tag{3}$$

III. RESULTS AND DISCUSSION

Figure 1 shows a plot for the potential in the r-z plane of a InGaN/GaN truncated-cone QD. The height of the QD and the diameters of the circles at the bottom and the top are fixed to be 4.0 nm, 5.0 nm, and 3.0 nm, respectively. There is a large potential difference between the top and the bottom of the QD, which leads to a spatial separation of the electron and hole wavefunctions because the electrons and the holes are attracted towards the top of the QD and the bottom of the QD, respectively. In Fig. 2, we plot the strain field along the z-axis of a InGaN/GaN truncated-cone QD with a wetting layer thickness of 1.0 nm. In the case of the strain fields along the z-axis, the shear strains ϵ_{xy}, ϵ_{yz}, and ϵ_{xz} are very small because of the rotational symmetry, which is not shown here. However, in general, the shear strains are not negligible along directions lacking such a symmetry. The misfit strain, ϵ_0, of the QD is taken with respect to the surrounding matrix so that the QD is initially strained by ϵ_0 = -0.020 in the z-direction and ϵ_0 = -0.022 in the x- and the y-directions. The initial strain is taken as negative for a material under compression. The biaxial compressive strain ϵ_{zz} occurs due to the surrounding material forcing the QD to assume the c-plane lattice constant of GaN. This is accompanied by an extension, indicated by a peak of ϵ_{zz} in the QD, observed at 25 Å along the z-axis. On the other hand, ϵ_{zz} becomes tensile in the surrounding matrix because the QD exerts the opposite force on the surrounding matrix.

Figure 3 shows the potential along the z-axis of a InGaN/GaN truncated-cone QD with a wetting layer thickness of 1.0 nm. The internal field is determined from the difference between the sum of the spontaneous and the piezoelectric fields in the QD and that in the barrier. Thus, the relative contributions of the strain-induced and the spontaneous potentials to the total potential depend on the material compositions. In the case of InGaN/GaN QDs, the potential is observed to be almost entirely contributed by the strain-induced piezoelectric polarization, irrespective of the In composition. The weak spontaneous potential in InGaN/GaN QDs is due to the small difference in the spontaneous polarization constants of the two materials. The potential is shown to be maximum near the boundary between the QD region, including the wetting layer, and the barrier region. The strain-induced potential rapidly increases with increasing In composition. For example, the strain-induced potentials at the boundary are 0.37 and 0.91 for QDs with $x = 0.2$ and 0.6, respectively.

Figure 4 shows the potential along the z-axis for these wetting layer thicknesses of a InGaN/GaN truncated-

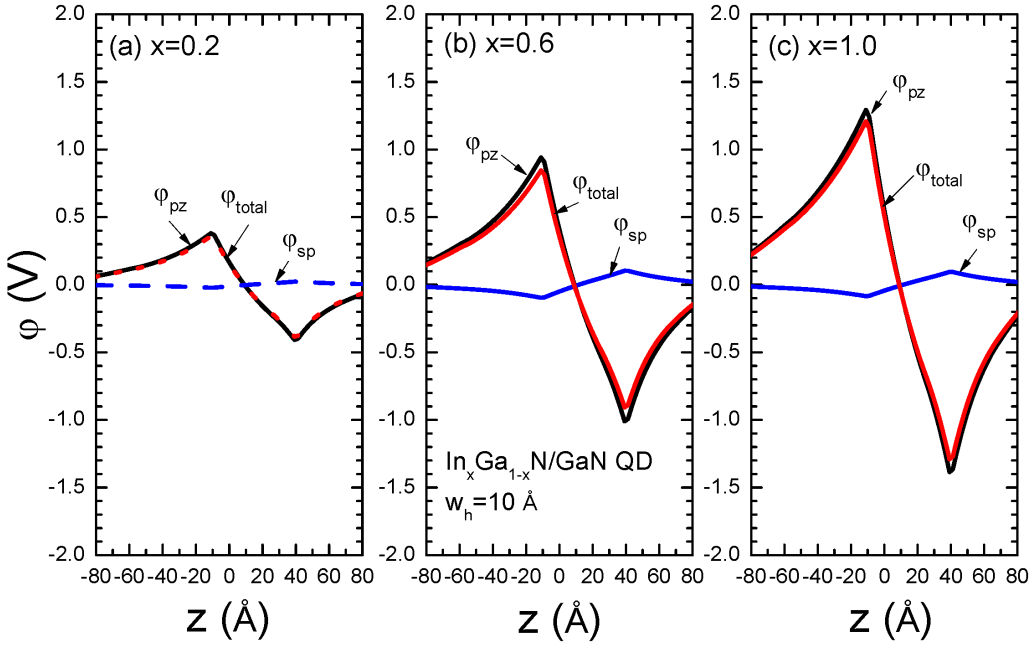

Fig. 3. (Color online) Potential along the z-axis of a InGaN/GaN truncated-cone QD for three values of x with a wetting layer thickness of 1.0 nm.

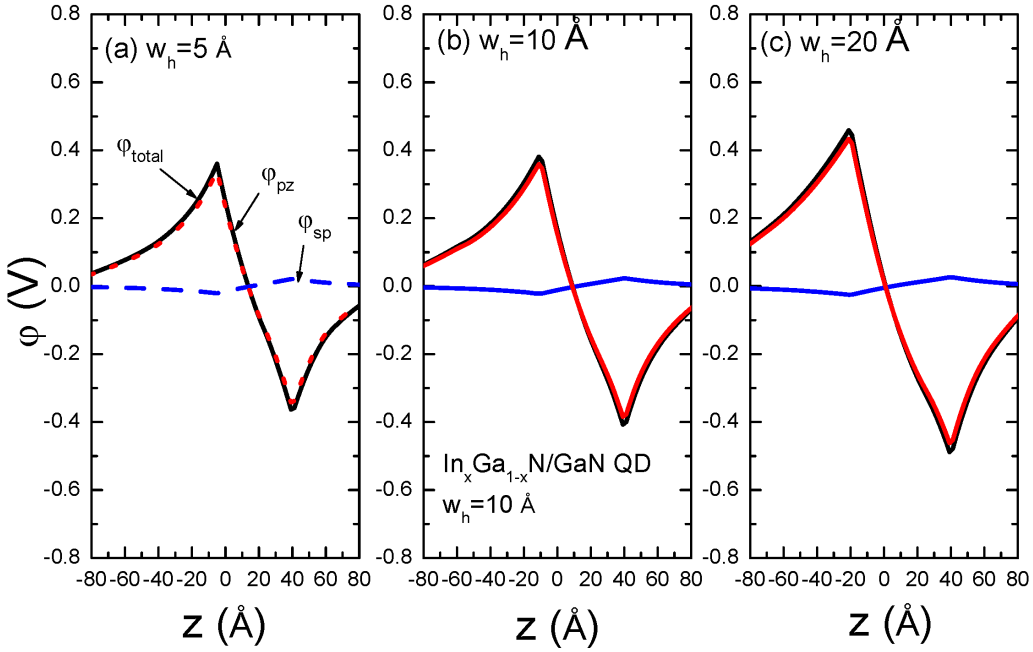

Fig. 4. (Color online) Potential along the z-axis for three the wetting layer thicknesses of a InGaN/GaN truncated-cone QD with $x = 0.2$.

cone QD with $x = 0.2$. The total potential at the boundary between the QD and the barrier regions gradually increases with increasing wetting layer thickness. This can be explained by the fact that, if the internal field is constant in the QD, the potential is given by the product of the electric field and the height of the QD along the z-axis. That is, the potential along the z-axis increases because the total width of the QD along the z-axis increases with increasing wetting layer thickness. The increase in the total potential at the boundaries leads to a larger potential difference between the top and the bottom of the QD. Hence, it the interband transition energies are expected to be redshifted and the optical matrix elements representing the transition probability between the electron and the hole states are expected to be reduced with increasing wetting layer thickness.

IV. SUMMARY

In summary, the polarization potentials as functions of the wetting layer thickness and the In composition in InGaN/GaN semiconductor QDs are investigated using the theory of continuum elasticity and a FEM method. In the case of the strain fields along the z-axis, the shear strains ϵ_{xy}, ϵ_{yz}, and ϵ_{xz} are found to be very small. The strain-induced potential rapidly increases with increasing In composition. The potential is almost entirely contributed by the strain-induced piezoelectric polarization, irrespective of the In composition. The total potential at the boundary between the QD and the barrier regions gradually increases with increasing wetting layer thickness. Thus, the optical properties are expected to depend highly on the wetting layer thickness.

ACKNOWLEDGMENTS

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2009-0071446).

REFERENCES

[1] G. Martin, A. Botchkarev, A. Rockett and H. Morkoç, Appl. Phys. Lett. **68**, 2541 (1996).
[2] F. Bernardini, V. Fiorentini and D. Vanderbilt, Phys. Rev. B **56**, 10024 (1997).
[3] D. P. Williams, A. D. Andreev, E. P. O. Reilly and D. A. Faux, Phys. Rev. B **72**, 235318 (2005).
[4] M. Arley, J. L. Rouviere, F. Widmann, B. Daudin, G. Feuillet and H. Mariette, Appl. Phys. Lett. **74**, 3287 (1999).
[5] F. Boxberg and J. Tulkki, Rep. Prog. Phys. **70**, 1425 (2007).
[6] W. P. Hong and S. H. Park, J. Korean Phys. Soc. **55**, 1607 (2009).
[7] W. P. Hong and S. H. Park, J. Korean Phys. Soc. **55**, 2496 (2009).
[8] Y. W. Kwon and H. Bang, *The Finite Element Method Using Matlab* (CRC Press, New York, 2000).