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Built-in electric fields and electronic structure of GaN/AlN QDs

A. D. Andreev† and *E. P. O'Reilly*‡
† Ioffe Physico-Technical Institute, St Petersburg, Russia
‡ Physics Department, University of Surrey, Guildford, GU2 5XH, UK

Abstract. We present a theory of the electronic structure of GaN/AlN QDs including built-in strain and electric field effects. A simple analytical formula is derived for the Fourier transform of the built-in electrostatic potential. The QD carrier spectra and wave functions are calculated using an original method we have developed based on an 8-band **k·P** model. It is shown that due to the strong built-in electric field, the holes are localized in the wetting layer just below the QD bottom, while electrons are pushed up to the pyramid top. The energy of the ground optical transition is found to be in good agreement with available experimental data.

Introduction

Wide-bandgap nitride-based quantum well (QW) and dot structures have significantly different properties compared to the "classical" GaAs-based QW and QD structures. Whereas GaAs and most other III–V compounds have a cubic (zinc-blende) crystal structure, GaN and related nitride alloys generally have a hexagonal (wurtzite) structure, which leads to strong built-in piezoelectric fields in heterostructures, of the order of MV/cm. As a consequence, self-organized GaN/AlN QDs can exhibit a large red shift in the energy of the photoluminescence maximum, with interband emission reported about 0.5 eV below the GaN bulk bandgap [ ].

The main aim of this paper is to study theoretically the influence of built-in electric fields on the electronic structure of hexagonal GaN/AlN QD structures and to compare the results with available experimental data. To the best of our knowledge, we present the first theoretical investigation of the carrier states in GaN-based QDs, which we carry out in the framework of a multi-band $\mathbf{k} \cdot \mathbf{P}$ model, including the effects of the 3D strain and built-in electric field distributions.

1. Built-in strain and electric fields

The calculation of the spatial strain distribution in a QD structure requires the solution of a 3D problem in elasticity theory, often for a non-trivial quantum dot shape. In this paper we introduce a novel approach based on a Green's function tensor formalism to calculate the 3D strain distribution in QD structures of arbitrary shape, and with hexagonal crystal symmetry. We derive an analytical expression for the Fourier transform of the QD strain tensor, valid for the case when the elastic constants of the QD and matrix materials are equal. We then obtain a compact analytical expression for the Fourier transform of the strain tensor. The 3D spatial distribution of the strain tensor is then found easily as the sum of the Fourier series.

A schematic 3D view of the GaN/AlN QD considered in this paper is shown in Fig. 1(a), with cross-section shown in Fig. 1(b) (view in x-z plane). In the calculations below, the shapes of the QDs are as presented in Fig. 1, with the sizes and vertical repeat distances

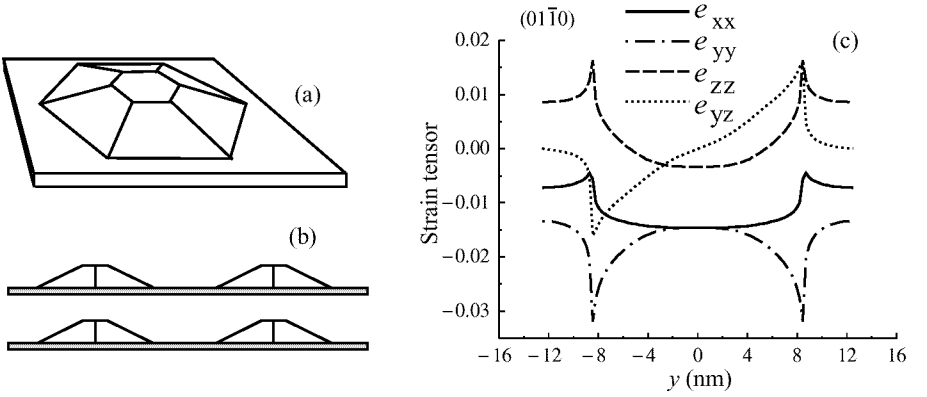

Fig. 1. Showing schematic diagrams of GaN/AlN QDs shaped as truncated hexagonal pyramids (a) 3D view of a single QD standing on a wetting layer; and (b) view of the QD structure in the x-z plane. (c) Position dependence of the strain tensor components along the (01$\bar{1}$0) direction, $x = z = 0$.

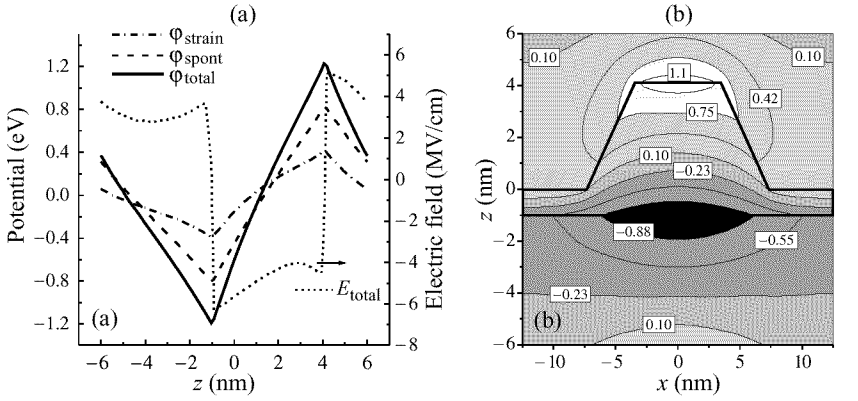

Fig. 2. (a) Calculated variation of the built-in electrostatic potential components, φ, and total electric field, E, along the (0001) direction ($x = y = 0$). Solid line: Total built-in electrostatic potential, φ_{total}, found as the sum of the strain-induced piezoelectric potential, φ_{strain}, (dot-dashed line) and the spontaneous polarisation term, φ_{spon} (dashed line). (b) Contour plot of the variation in the total built-in electrostatic potential, φ_{total} in the x-z plane ($y = 0$). The darkest areas show regions of low potential (where holes are trapped), and the brighter areas regions of higher potential (where electrons are trapped). The numbers in boxes show the magnitude of the potential (in eV) along the different contour lines.

used taken from experimental data [2]. Figure 1(c) shows the calculated variation of the strain tensor components along the (01$\bar{1}$0) direction. The magnitudes of the the strain fields peak near the pyramid edges, with smoother variations away from the edges. We have used a similar technique to calculate the Fourier transform of the built-in electric field, including the strain-induced piezoelectric field and the contribution due to the spontaneous polarization. The two sets of field terms give approximately equal contributions to the calculated built-in electric field in GaN/AlN QD structures, where the overall electric field magnitude can be of the order of several MV/cm. For example, using the piezoelectric

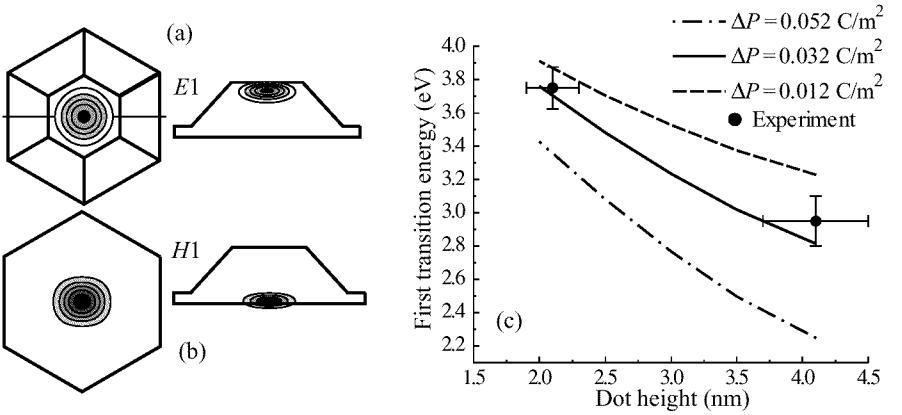

Fig. 3. Probability density distribution, $|\Psi(\mathbf{r})|^2$ for the first electron (a) and hole (b) states in the GaN/AlN QD. (c) Calculated dependence of the ground state transition energy E1-H1 on QD height for different assumed values of the spontaneous polarization difference, $\Delta P_{\text{spont}} = P_{\text{QD}} - P_{\text{M}}$.

constants and spontaneous polarization values predicted by Bernardini *et al.* [3], we find the electric field in a GaN/AlN QD of height 4.1 nm to be around 6 MV/cm at the QD base and 4 MV/cm at the QD top (see Fig. 2(a)). Such giant built-in electric fields are characteristic for GaN/AlN QD structures.

2. Electronic structure

We use an efficient technique to calculate the carrier energy spectrum and wave functions in a semiconductor heterostructure containing QDs of arbitrary shape. The method is a natural combination of the plane-wave expansion and Fourier transform techniques used to derive the built-in strain and electric field distributions. Each carrier wave function is expressed in a series expansion based on a suitable set of bulk states. The coefficients of the series and the carrier energy levels in any QD are then found as the eigenvectors and eigenvalues of a Hamiltonian matrix, all of whose matrix elements can be found analytically. The proposed technique does not require explicit calculation of the 3D spatial distribution of the built-in strain and electric fields. This makes the method effective and fast not only for spectrum calculations, but also for further modeling of the optical properties of the QD structures.

The built-in electric field has a crucial influence on the carrier states in GaN/AlN QDs. The electrons are pushed up to the QD top and holes are pushed down into the wetting layer below the QD. In addition, both electrons and holes experience a significant lateral confinement due to the built-in electrostatic potential (see Fig. 2(b)). This creates an effective 3D potential for electrons and holes, with flat, circular symmetry. The form of the electron and hole wavefunctions in GaN/AlN QDs is therefore very similar to what would be expected for an infinitely deep flat cylinder (see Fig. 3(a,b)).

Finally, the calculated dependence of the energy position of the first PL maximum on QD size is found to be in good agreement with two experimental points from [1] for "large" and "small" GaN/AlN QDs (heights respectively ~4 nm and 2 nm), if we assume that the difference between the spontaneous polarization values of GaN and AlN, $\Delta P_{\text{spont}} \approx 0.032$ C/m^2 (see Fig. 3(c)). This value of ΔP_{spont} is ~40% smaller than the one of 0.052 C/m^2 calculated by Bernardini, *et al.* [3], but is consistent with other experimental data and analysis on GaN/AlGaN heterostructures [4, 5, 6]. We conclude

that the method introduced here gives valuable information on the electronic structure of GaN/AlN quantum dots, and should also be particularly convenient for a range of future studies, including modeling of optical transition rates, and laser gain characteristics of realistic quantum dot structures.

Conclusion

In conclusion we note that the technique which we present here for calculation of the built-in electric and strain fields in semiconductor structures with QDs of arbitrary shape can also be applied to other structures based on a variety of compounds like GaAs/InAs, InP and ZnSe/CdSe.

Acknowledgements

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