A simple model for conduction band states of nitride-based double heterostructures

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Abstract. In this work we propose an analytical expression for the approximate modeling of the potential energy function describing conduction band bending in III-V nitride quantum wells. It is an alternative approach to the self-consistent Poisson-Schrodinger calculation. The model considers the influence of the many electron system and the built-in electric field inside the well. Hartree and exchange contributions are included along the lines of a local-density Thomas-Fermi-based theory. The effects due to the modulated doping in the barriers is also considered. We report the calculation of the energy spectrum as a function of several input parameters: alloy composition in the barriers, barrier doping concentration, and quantum well width. Our results could be of usefulness in the study of optoelectronic properties in this kind of systems.

1. Introduction

The wurtzite nitrides exhibit high values of the piezoelectric constants as well as large spontaneous polarizations due to their lack of central symmetry in the crystal unit [1, 2, 3, 4, 5]. This fact has a consequence of special interest: the formation of two-dimensional charge densities at the interfaces, when a heterostructure made of these materials is formed. This kind of charge density is induced by the electric polarization resulting from the superposition of the spontaneous and piezoelectric polarization fields of both materials across each interface.

In the particular case of heterostructures, large built-in electric fields form in wurtzite III-V nitrides thin films and multilayers. Such fields originate from heterointerface discontinuities of the macroscopic bulk polarization of the nitrides [6, 7]. It has been found that the strain and the strain-induced piezoelectric field significantly alter the subband structure [8, 9]. For instance, the optical properties of GaInN/GaN/AlGaN quantum wells are governed to a large extent by the spontaneous and piezoelectric polarization fields arising from the strongly polar nature of wurtzite nitrides. In multiple quantum wells the electric fields lead to spatially highly indirect transitions between nearest and next nearest neighbour quantum wells [10]. On the other hand, there are some works in which it is shown that of the macroscopic polarization fields can be screened via modulation doping in nitride quantum wells [11].

In this work we present a simple analytical formulation describing the one-dimensional conduction band potential profile in nitride-based quantum wells with the prototype AlGaN/GaN/AlGaN. The presence of polarization-induced interface charge densities as well as the influence of intentional doping in the barrier regions are explicitly taken into account in
deriving the confining potential function. In the derivation, the one-dimensional local density Thomas-Fermi approach is used to generate the expression for the quantum well bottom profile.

2. Model and results

Let us assume that the polarization-induced surface charge densities at the interfaces of the AlGaN/GaN quantum well are given by \( \sigma_1 \delta(z) \) and \( \sigma_2 \delta(z - l_{qw}) \), where \( l_{qw} \) is the width of the well region. In addition, two selectively doped regions with three-dimensional ionized donor impurity density \( N_d \), are created in both AlGaN barriers, separated from the well interfaces via spacer layers of width \( d \). That is, the region located at the left of \( z = 0 \) extends from \( z = -d \) to \( z = -L_1 - d \). The doped region located at the right of \( z = l_{qw} \) extends from \( z = l_{qw} + d \) to \( z = L_2 + l_{qw} + d \). Both doped regions will have their respective width lengths \( L_1 \) and \( L_2 \) given by the depletion approximation. Taking into account these density charge distribution in the system, the proposed form for the potential function in the system is derived using the method presented in refs. [12, 13]:

\[
V(z) = \begin{cases} 
V^I_b, & z \leq -L_1 - d; \\
4\pi \frac{\varepsilon}{\varepsilon_{AlGaN}} N_d (d + L_1 + z)^2 + V^I_b, & -L_1 - d \leq z \leq -d; \\
8\pi \frac{\varepsilon}{\varepsilon_{GaN}} N_d L_1 (d + \frac{L_1}{2} + z) + V^I_b, & -d \leq z \leq 0; \\
- \frac{V^I_q}{(\frac{\eta}{\varepsilon_{AlGaN}} z + 1)^4} - \frac{V^{II}_{qw}}{(\frac{\eta}{\varepsilon_{GaN}} (l_{qw} - z) + 1)^4}, & 0 \leq z \leq l_{qw}; \\
8\pi \frac{\varepsilon}{\varepsilon_{AlGaN}} N_d L_2 (d + \frac{L_2}{2} + z) + V^{II}_b, & l_{qw} \leq z \leq l_{qw} + d; \\
4\pi \frac{\varepsilon}{\varepsilon_{GaN}} N_d (-d + L_2 - l_{qw} + z)^2 + V^{II}_b, & l_{qw} + d \leq z \leq l_{qw} + d + L_2; \\
V^{II}_b, & z \geq l_{qw} + d + L_2.
\end{cases}
\]

In this expression all the quantities are expressed in effective atomic units (Rydberg energy and Bohr radius) related with the GaN. In this sense, \( \varepsilon = \epsilon_{AlGaN}/\epsilon_{GaN} \) has the meaning of a relative dielectric constant, whereas;

\[
\eta = \frac{2}{15\pi} \quad \text{and} \quad z_{oj} = \left( \frac{\eta^3}{2\pi N^j_{eff}} \right)^{1/5}, \quad N^j_{eff} = \sigma_j + N_d L_j ;
\]

where the index \( j \) labels barrier regions \( I \) and \( II \). The amplitudes of the Thomas-Fermi potentials that combine within the well region are given by:

\[
V^j_{qw} = \frac{\eta^2}{z^4_{oj}}.
\]
To specify the set of undetermined constants appearing in equation (1), it is necessary to impose certain restrictive conditions. In first place, we must obtain that for \( z = 0 \) and \( z = l_{qw} \), the height of the barrier is equal to \( V_o \), which is no other than the value for the conduction band offset in the heterostructure, provided the origin for the energy is taken at the conduction band bottom in the GaN layer. With this in mind, it is found that:

\[
V^j_b = V_o - \frac{8\pi}{3} N_d L_j \left( \frac{L_j}{2} + d \right) - V^i j_{qw} - \frac{V^j_{qw}}{\left( \frac{n}{z_o l_{qw} + 1} \right)^4} \tag{4}
\]

The second set of restrictions are related to the charge conservation in the structure. This is attained if:

\[
V'(z_{l_k}^-) - V'(z_{l_k}^+) = \frac{4\pi}{\varepsilon} \sigma_k, \quad k = 1, 2. \tag{5}
\]

The points at which the derivatives of the potential are evaluated are \( z_{l_1} = 0 \), and \( z_{l_2} = l_{qw} \). This conditions determine, self-consistently, the values of the depletion lengths \( L_1 \) and \( L_2 \).

Now we discuss some properties of the potential function derived with this scheme.

- It is obvious that \( \sigma_1 \neq \sigma_2 \). They are going to be equal only when \( l_{qw} \rightarrow \infty \). Both 2D charge densities depend upon the strain, and this changes depending on which material the substrate layer is made up, and on the value of its width.
- The value of the built-in electric field inside the well is

\[
V(0^+) - V(l_{qw}^-) = -V_{qw}^I - \frac{V_{qw}^{II}}{\left( \frac{n}{z_o l_{qw} + 1} \right)^4} + \frac{V_{qw}^I}{\left( \frac{n}{z_o l_{qw} + 1} \right)^4} + V_{qw}^{II}. \tag{6}
\]

This will be equals to zero when \( l_{qw} \rightarrow \infty \), due to we have \( \sigma_1 = \sigma_2, L_1 = L_2 \), and \( z_{oI} = z_{oII} \). In this limit we recover the potential profile of two isolated single heterostructures.

At this point it is convenient to state that this model is also valid in the case of modulation-doped double heterostructures with no polarization-induced built-in intrawell electric fields associated. In that case, we could set, for instance, \( \sigma_1 = \sigma_2 = N d_L (L_1 = L_2) \) from the beginning. Under such condition, the obtained potential well profile is completely symmetric, with \( V'(l_{qw}/2) = 0 \).

Figure 1 shows the potential well profile, given in units of \( 10^{-3} \) eV, for a AlN/GaN/AlN double heterostructure. It has been assumed that the barriers are homogeneously doped with a donor concentration of \( N_2 = 5 \times 10^{18} \) cm\(^{-3} \) [12]. Besides, the strain relaxation parameter is taken to be unity [13]. Three different values of the well width are considered: 100, 150, and 200 \( \AA \). It can be seen that the value of the internal electric field is significantly dependent on that parameter as predicted in equation (6).

### 3. Conclusions

In this work we have presented a model analytical proposal for the description of conduction band bending in nitride double heterostructures. Together with its simplicity, it provides appropriate limiting cases as well as an expression for the built-in electric field in the quantum well. A previous version of this model, applied to nitride single heterostructures have proven to be a reliable and quite accurate approach to provide very good quantitative agreements with detected single electron states in AlGaN/GaN field effect transistors [14]. Therefore, it is of interest to continue exploiting the approach here introduced. The results of that work will be published later on.
Figure 1. Potential well profile (in meV) as a function of the position (in Å) for a AlN/GaN/AlN double heterostructure, derived within the model proposed in the present article. Values of the well width included are 100, 150, and 200 Å.

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