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Tunnelling and current density in short period strained AlN/GaN superlattices

Iglika Asenova*, Evgenia Valcheva, Dimo Arnaudov

Department of Physics, Sofia University, 5 James Bourchier Blvd, 1164 Sofia, Bulgaria

HIGHLIGHTS

- We model strained AlN/GaN superlattice by means of transfer matrix formalism.
- We calculate the transmission coefficient and the tunnel current density.
- Broadening, destroying and regrouping of the minizones are observed.
- Oscillation behavior of the tunnel current is observed.
- Conductance calculations are in agreement with the experimental data.

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ABSTRACT

In this paper we theoretically analyze the under-barrier perpendicular transport in short period strained III-nitride superlattices via a generalized model. The transmission coefficient of unbiased and biased structures, as well as the tunnel current at room temperature, are calculated via the transfer matrix formalism and the effective mass approximation. The inherent to the III-nitrides electric polarization fields taken into account and the exact solution of the Schrodinger equation is used in the calculation process. The minizone structure is shown to periodically disintegrate and reform as the externally applied electric field increases, while the tunnel current density shows nonlinear behavior and negative differential conductance. The theoretical results we obtain are compared and found to be consistent with the experimental ones.

1. Introduction

The III-nitride heterostructures, multiple quantum wells (MQWs) and superlattices in particular, have attracted much interest in the recent years as promising candidates to be used in device technology [1,2]. Few of their numerous applications include devices for the optical communication region, high electron mobility transistors, ultra-violet lasers, light emitting diodes, and resonant tunnelling based structures for THz applications [3–10]. The recent progress in constructing intersubband devices based on III-nitride quantum wells, requires extensive studies [11,12] on the subject. The main operating principles in the superlattice devices are the tunnelling processes [13,14], which have been studied the recent decades both theoretically and experimentally. Appealing from analytical and practical point of view, considerable part of the theoretical approaches for studying tunnelling process is based on the transfer and the scattering matrix formalism [15–19].

In the III-nitride barrier devices the semiconductor layers are usually grown in the wurtzite modification, since it is the thermodynamically stable structure for ambient conditions. Numerous researches have shown that the macroscopic spontaneous and piezoelectric polarization, peculiar to the wurtzite modification, significantly affect the optical and electronic properties of the layered structures [20–22] even in the absence of bias. Studying the electronic and conduction properties of III-nitride wurtzite barrier structure implies taking account not only of the bias, but also of the in-layer electric fields. Studies of the transmission through III–V MQWs, applicable for three and five barriers, and based on the scattering matrix formalism, were previously reported [23–25].

In this work we present a generalized model based on the transfer matrix (T-matrix) formalism and the effective mass approximation for *N*-period strained wurtzite AlN/GaN superlattice in tunnelling regime, while taking account of the in-layer electric fields and the bias. As the in-layer polarization fields change significantly the potential profile of the structure and in

* Corresponding author.
E-mail address: iasenova@phys.uni-sofia.bg (I. Asenova).

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order to do the calculations with an adequate accuracy, we consider the exact solution of the Schrodinger equation, provided by the Airy functions. Avoiding the exact solution and using approximating techniques, such as the WKB approximation, is not recommended when calculating tunnel current through trapezoidal barrier. It was shown in a previous study [26] that this calculation requires the exact solution of the Schrodinger equation, otherwise the oscillation behavior of the tunnel current may not be observed.

The matrices we use for our calculations are related, according to the accepted classification [27–29], to the second kind of T-matrices. We study the perpendicular below-barrier transmission properties of the superlattice, and the tunnel current as well. The original heterostructures, that inspired our research, are presented in a study [30], where their photoluminescent properties are examined. Our intention is to study the tunnelling of biased and unbiased 10 period AlN/GaN superlattice, as well as to analyze the oscillation behavior of the tunnel current, which was previously observed experimentally [31]. The transmission coefficient in tunnelling regime is calculated in range of parameters such as layer thickness, in-layer polarization fields and bias. A comparison between the experimental and the calculation results is provided for the conductance-voltage characteristic. Both of them reveal regions of negative differential conductivity.

The paper is organized as follows. In Sections 2 and 3 we give a detailed derivation of the T-matrix for biased barrier structure and present the material parameters we are working with. In Section 4 we present the transmission coefficient, the tunnel current, as well as a comparison between the experimental and theoretical results, and discuss our calculations. In the concluding Section 5 we summarize the results and make some general remarks.

2. Theoretical framework

A superlattice is obtained by alternatively arranging layers of wider-gap and narrower-gap semiconductor materials. We consider ideal periodic structure constituted of $N+1$ layers of wider gap material alternating with N layers of narrow gap material, which represent potential barriers and wells respectively. In this study we consider the offset and the profile in the conduction band only. The offset equals the difference in the electronic affinities of the contacting materials, according to the Andersons model. The miniband structure can be derived by solving the Schrodinger equation for the one-dimensional periodic potential along the growth direction of the superlattice – in this case the wurtzite [0001]. In order to do that, we assume previously introduced simplifications [32], i.e. the electron is characterized by an isotropic effective mass and the scattering effects are to be neglected.

Since the examined structure is composed of thin layers wurtzite AlN and GaN, we have to take into consideration the macroscopic electric polarization that is inherent to the III-nitride materials and is strongly displayed near the heterointerfaces [22]. The total polarization in the well (GaN) and barrier (AlN) regions is the sum of the spontaneous and the piezoelectric components. The former is always directed along the $[000\bar{1}]$ axis, while the latter is directed either along or opposite to the [0001] axis, depending on the lattice mismatch strain. The resulting electric fields are calculated to be [22]

$$\mathbf{E}_w = \frac{(\mathbf{P}_b - \mathbf{P}_w)L_b}{(\varepsilon_b L_w + \varepsilon_w L_b)\varepsilon_0} \tag{1}$$

$$\mathbf{E}_b = \frac{(\mathbf{P}_w - \mathbf{P}_b)L_w}{(\varepsilon_w L_b + \varepsilon_b L_w)\varepsilon_0} \tag{2}$$

for the well (w) and the barrier (b) regions respectively. In the above expression the total polarization in the layers is represented by $\mathbf{P}_w$ and $\mathbf{P}_b$, while L_w and L_b denote their width and thickness, ε_w and ε_b are the relative permittivities of the materials, ε_0 is the vacuum permittivity.

For the sake of our calculations, we choose a spatial variable z along the growth direction of the superlattice and we set $z_1 = 0$ to be the left boundary of the 1-st barrier. In terms of L_w and L_b, the left and the right boundary of the n-th barrier are $z_{2n-1} = (n-1)(L_b + L_w)$ and $z_{2n} = nL_b + (n-1)L_w$ respectively. In unbiased III-nitride superlattice, due to the in-layer polarization fields from (1) and (2), the potential wells and barriers assume the corresponding trapezoidal form of $-eE_w z$ and $eE_b z$, e being the electron charge. If external electric field E_{ext} is applied, it will be superimposed over the trapezoidal wells and barriers. Thus, the potential profile of the structure will be described by the following relations:

$$U_{wn} = neE_w(L_w + L_b) - e(E_w + E_{ext})z \quad \text{where } n = 1, \ldots, N \tag{3}$$

$$U_{bn} = U_0 - (n-1)eE_b(L_w + L_b) + e(E_b - E_{ext})z \quad \text{where } n = 1, \ldots, N+1 \tag{4}$$

for the wells and the barriers respectively. In the above expressions U_0 denotes the conduction band offset. The potential profile along the growth direction of biased and unbiased structure is shown on a not-to-scale graphic in Fig. 1.

The one-dimensional Schro dinger equation for the regions of the wells and the barriers respectively takes the form:

$$\left(-\frac{\hbar^2}{2m_w^*}\frac{d^2}{dz^2} + U_{wn}\right)\psi_n^{(w)}(z) = \varepsilon\psi_n^{(w)}(z) \quad \text{where } n = 1, \ldots, N \tag{5}$$

$$\left(-\frac{\hbar^2}{2\,m_b^*}\frac{d^2}{dz^2} + U_{bn}\right)\psi_n^{(b)}(z) = \varepsilon\psi_n^{(b)}(z) \quad \text{where } n = 1, \ldots, N+1, \tag{6}$$

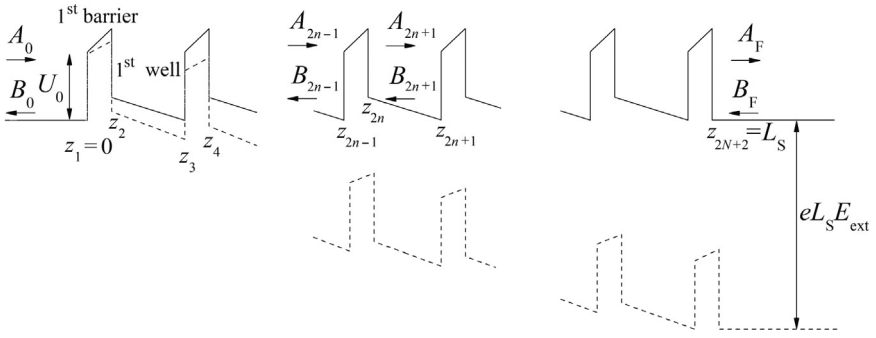

Fig. 1. Potential profile of unbiased (solid line) and biased (dashed line) AlN/GaN superlattice with N wells (GaN layers) and $N+1$ barriers (AlN layers). The in-layer polarization fields $\mathbf{E}_w$ and $\mathbf{E}_b$ are responsible for the trapezoidal shape of the potential wells and barriers of the unbiased profile.