Polarization dependence of III-nitride superlattice transmission coefficient

I S Asenova and E P Valcheva
Faculty of Physics, Sofia University, 5 J. Bourchier Blvd, Sofia, Bulgaria
E-mail: iasenova@phys.uni-sofia.bg

Abstract. We study the tunnelling process and behaviour of the transmission coefficient of an AlN/GaN superlattice as the internal polarizations in the composing layers change. Our calculations are based on the transfer matrix formalism and the exact solution of the Schrödinger’s equation provided by the Airy functions. We also examine the dependence between the minizones width and the magnitude of the internal polarizations both for unbiased and biased structure.

1. Introduction

According to the recent researches [1], the III-nitride layered heterostructures have shown promising features for the manufacturing of devices for the optical communication region, high electron mobility transistors, ultra-violet lasers and resonant tunneling based structures for THz applications [1,2,3]. It has also bee shown that the internal piezo- and pyroelectric polarizations of the wurtzite modification have a significant effect upon the electronic properties of the barrier structures [4].

The calculations and the results we present here are inspired by the sample provided in [5] and are based on a previously presented model [6]. We use the effective mass approximation and the transfer matrix formalism. Our purpose is to demonstrate the behaviour of the transmission coefficient and the minizones in the conduction band for a ten-period wurtzite AlN/GaN superlattice in and out of the presence of external homogeneous electric field, while theoretically modifying the actual magnitudes of the polarizations in the layers. To assure a desired accuracy, we use the Airy function formalism when solving the one-dimensional Schrödinger’s equation for the superlattice potential [7].

2. Theoretical framework

The superlattice we are interested in is composed of 11 layers wide-gap semiconductor material, i.e. AlN, which alternates with 10 layers of narrow-gap semiconductor material, i.e. GaN, and we examine the one-dimensional potential along the z-axis. The discontinuity in the conduction band of the contact materials is represented by \( U_0 \). On account of the internal, i.e. both piezoelectric and pyroelectric, polarization of the layers, the profiles of the wells and the barriers will not be rectangular even in the bias-free case. Instead, they assume trapezoidal form due to the internal electric fields, whose magnitudes are calculated as follows:

\[
E_{w,b} = \frac{\left( P_{b,w} - P_{w,b} \right) L_{b,w}}{\left( \varepsilon_{b,w} L_{w,b} - \varepsilon_{w,b} L_{b,w} \right) \varepsilon_0}
\]  

(2.1)
in the wells and barriers regions, respectively. Here \( P_{w,b} \) represents the total polarization in the layer, \( L_{w,b} \) – its thickness, \( \varepsilon_{w,b} \) – the relative permittivities of the alternating well and barrier materials respectively, and \( \varepsilon_0 \) is the vacuum permittivity. Thus, the actual height of the potential barrier is defined to be:

\[
U = U_0 + eE_b L_b,
\]

where \( e \) is the elementary charge.

The bias, when applied, will further influence the potential profile of the structure. According to the direction we have chosen, the magnitude of the local field will increase the well regions and decrease in the barrier regions, as follows:

\[
U_{w_n} = neE_w (L_w + L_b) - e(E_w + E_{\text{ext}})z
\]

\[
U_{b_n} = U_0 - (n-1)eE_b (L_w + L_b) + e(E_b - E_{\text{ext}})z
\]

in the \( n \)-th well and the \( n \)-th barrier, respectively. Here \( E_{\text{ext}} \) represents the magnitude of the external field. In our model, the bias is applied between the first and the last barrier, i.e. from \( z = 0 \) to \( z = L_{\text{tot}} = 10(L_w + L_b) + L_b \). A not to scale graphic, depicting the potential profile in the conduction band of biased and nonbiased structure, is shown on figure 1.

Figure 1. A not to scale graphic of the potential profile along the \( z \)-axis of biased (dashed line) and nonbiased (solid line) superlattice.

The solutions of the Schrödinger’s equation, i.e. the wave functions for the one-dimensional potential of the superlattice considered, are given by the Airy functions and are presented in a previous study [6]. Outside the superlattice, the wave functions are represented by plane waves. We consider the incident and the reflected component of the wave functions at each interface and impose the effective mass dependent boundary conditions [8]. Thus we define \( 2 \times 2 \) transfer matrices to correlate the amplitudes of the wave function on the right and on the left of each barrier and we are able to construct a transfer matrix for the multi-barrier system as follows:

\[
\begin{pmatrix}
A_F \\
B_F
\end{pmatrix} = [R] \prod_{n=2}^{10} \begin{pmatrix}
T & \frac{1}{(12-n)} \\
L & 0
\end{pmatrix} \begin{pmatrix}
A_0 \\
B_0
\end{pmatrix} = [\Omega] \begin{pmatrix}
A_0 \\
B_0
\end{pmatrix}.
\]

(2.5)

Here \( A_0 \) and \( B_0 \) are the amplitudes of the wave function in the region \( z < 0 \), \( A_F \) and \( B_F \) are the amplitudes for \( z > L_{\text{tot}} \), \( [R] \) and \( [L] \) are the transfer matrices for the rightmost and the leftmost
The transfer matrices for each of the other barriers and \( \Omega \) represents the \( 2 \times 2 \) transfer matrix of the overall system. The particular components of each matrix are fully presented in [6].

In the case examined, the outgoing wave has no reflection component, i.e. \( B_y = 0 \) and the transmission coefficient is given by [9]:

\[
\tau = \frac{|A_F|^2}{|A_b|^2} = \left| \frac{\text{det}[\Omega]}{\Omega_{22}} \right| = \frac{1}{|\Omega_{22}|^2}. \tag{2.6}
\]

### 3. Numerical analysis

We calculate the below-barrier transmission coefficient on the basis of (2.6) for an AlN/GaN superlattice in range of internal polarizations and biases. We assume the conduction band discontinuity \( U_0 = 1.8 \text{eV} \) [5]; the internal polarizations \( P_w = -0.032 \text{C/m}^2 \) and \( P_b = -0.100 \text{C/m}^2 \) [10] in the well and the barrier, i.e. GaN and AlN layers, respectively; the relative permittivities \( \varepsilon_w = 9.5 \) and \( \varepsilon_b = 8.5 \) [1]; and the electron effective masses \( m^*_w = 0.22 m_0 \) and \( m^*_b = 0.30 m_0 \) [10], where \( m_0 \) is the electron mass. The electron effective masses outside the barrier structure, i.e. for \( z < 0 \) and \( z > L_A \) are chosen to equal \( m_0 \). The lattice constants of the well and barrier materials are \( c_{\text{GaN}} = 5.19 \text{Å} \) and \( c_{\text{AlN}} = 4.98 \text{Å} \) [1] respectively. The widths \( L_w \) and \( L_b \) of the wells and the barriers are defined by taking the number of unit cells equal to 9 and 3 respectively.

To examine the impact of internal polarizations on the transmission coefficient, we calculate the latter for ten, otherwise identical, superlattices that differ only in their internal polarizations. The magnitudes of the latter are modified by multiplying with suitable coefficients. The polarizations of the layers and the barrier heights of thereby generated structures are presented in table 1. The heights of the barriers are calculated after (2.1) and (2.2).

| Coefficient of multiplication | \( P_w \) (C m\(^2\)) | \( P_b \) (C m\(^2\)) | \( U \) (eV) |
|-------------------------------|------------------------|------------------------|-------------|
| 1.0                           | -0.0320                | -0.10                  | 2.75        |
| 0.9                           | -0.0288                | -0.09                  | 2.66        |
| 0.8                           | -0.0256                | -0.08                  | 2.56        |
| 0.7                           | -0.0224                | -0.07                  | 2.47        |
| 0.6                           | -0.0192                | -0.06                  | 2.37        |
| 0.5                           | -0.0160                | -0.05                  | 2.28        |
| 0.4                           | -0.0128                | -0.04                  | 2.18        |
| 0.3                           | -0.0096                | -0.03                  | 2.09        |
| 0.2                           | -0.0064                | -0.02                  | 1.99        |
| 0.1                           | -0.0032                | -0.01                  | 1.89        |

For the study of the transmission coefficient in presence of uniform external electric field, the values of the applied voltage are chosen to be 50 mV and 150 mV.

### 4. Results and discussion

To study the effect of the magnitude of the internal polarization in the layers upon the transmittance of the barrier structures, on figure 2 we present the transmission coefficients of the all ten nonbiased superlattices, whose features are listed above.
Figure 2. Bias free transmission coefficient ($\tau$) as functions of the incident electron energy. Each curve is labelled with the factor that multiplies the polarizations in the layers and is shifted along the vertical axis.

In all cases the transmission coefficient shows resonant peaks up to $\tau = 1$ and the resonant energies are grouped in five to six minizones. A tendency of lowering the position of each minizone as the magnitude of the polarization field lowers is clearly observed. The number of the quasi-levels in each minizone equals the number of the wells, i.e. ten, in the superlattice, which can be clearly observed in figure 2.

To study the effect of external electric field upon the transmittance for the superlattices considered, on figure 3 we present our calculations of the transmission coefficient for applied voltages of 50 mV and 150 mV.
Figure 3. Transmission coefficients ($\tau$) of biased superlattices as functions of the incident electron energy. Each curve is labelled with the factor that multiplies the polarizations in the layers and is shifted along the vertical axis. (a) For applied voltage of 50 mV. (b) for applied voltage of 150 mV.

As the bias grows the minibands are Stark shifted toward lower energies and tend to split. The transmission is suppressed in a greater degree for the miniband edge states than for the middle of the minizones. It is also more suppressed for the superlattices, whose layer polarizations are multiplied by a higher coefficient. The Stark shift exhibited by the resonant energies is greater for the lower band edge states than for the upper band edge states.

The change of the minizones width versus the magnitudes of the internal polarizations is presented on figure 4. The measurements are made for the three consecutive lowest minizones in case of nonbiased superlattice and are taken from the lowest to the highest quasi-level in each minizone.

Figure 4. Width of the lowest consecutive three minizones of nonbiased superlattice as a function of the coefficient that multiplies the polarizations in the layers. Each curve is labelled according to the minizone, whose width it represents.
It is shown that the lowest minizone exhibits the greatest narrowing as the magnitudes of the polarizations increase. While applying external electric field, it is observed that all minizones exhibit broadening, which is notably greater for the lower minizones than for the upper ones.

5. Summary
In this work the effect of the magnitude of the polarization in the layers of a barrier structure upon the transmittance is studied. The calculations are based on the transfer matrix approach and the Airy functions formalism. The transmission coefficients for ten identical, but in the layer polarizations, superlattices are presented, in and out of external homogeneous electric field. It is shown that the transmission coefficient is suppressed to a greater degree for the superlattices, whose layer polarizations are multiplied by higher coefficients. The rearrangement in the positions of the minizones is shown and the dependence between their width and the internal polarization magnitudes is demonstrated in the nonbiased case.

Acknowledgements
This work was partially supported by the National Science Fund of Bulgaria and by the French-Bulgarian Bilateral Program EGGIDE (PAI-RILA). We would also like to thank to the Faculty of Physics, Sofia University, Bulgaria for the financial support.

References
[1] Monemar B 1999 Journal of Materials Science: Materials in Electronics 10 227-254
[2] Cho A Y, Sivco D L, Hg H M, Gmachl C, Tredicucci A, Hutchinson A L, Chu S N G and Capasso F 2001 J. Cryst. Growth 227-228 1-7
[3] Camacho A S, Gutiérrez R M and Ardilla G 2005 Microelectronics Journal 36 922-927
[4] Ambacher O, Majewski J, Miskys C, Link A, M, Eickhoff M, Stutzmann M, Bernardini F, Fiorentini V, Tilak V, Schaff B and Eastman L F 2002 J. Phys.: Condens. Matter 14 3399-3434
[5] Valcheva E, Kirilov K, Monemar B, Amano H and Akasaki I 2009 Phys. Status Solidi C 6 S751-S754
[6] Asenova I, Valcheva E and Arnaudov D (in progress)
[7] Gundlach K H 1966 Solid-State Electronics 9 949-957
[8] Bastard G 1981 Phys. Rev. B 24 5693-5697
[9] Tsu R and Esaki L 1973 Appl. Phys. Lett. 22 562-564
[10] Vurgaftman I and Meyer J 2003 Journal of Applied Physics 94 3675-3696