

**ANALYTICAL MODELING OF TRANSMISSION COEFFICIENT OF $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaN}$ RESONANT TUNNELING DIODE IN PRESENCE AND ABSENCE OF ELECTRIC FIELD****Subhra Chowdhury¹, Dhrubes Biswas²**¹Advanced Technology Development Center, Indian Institute of Technology Kharagpur,
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Received 4-04-2012, accepted 10-04-2012, online 12-04-2012

ABSTRACT

$\text{AlGaIn}/\text{GaIn}$ Resonant Tunneling Diodes (RTD) have increasingly become important due to their high frequency performance and capability of providing negative differential resistance at room temperature. Transmission coefficient (Tc) is an important factor to determine the negative differential resistance (NDR) and peak-to-valley ratio of RTD. An analytical model is developed here to predict the variation of Tc of $\text{AlGaIn}/\text{GaIn}$ RTD structure using transfer matrix method. Variation of transmission coefficient with applied electric field is studied. Effect of barrier width and well width on transmission coefficient in presence and absence of applied electric field are also observed in this analysis. Dependence of conduction band discontinuity on composition of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier is also taken into account in the model.

Keywords RTD; $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaIn}$ RTD; Transmission coefficient; Applied electric field

I. INTRODUCTION

Recently, III-nitrides have gained interest for RTDs. Wide band gap, large conduction band discontinuity (~2.1 eV in AlN/GaIn) [1], high carrier mobility and thermal stability promise high power high frequency room temperature (RT) operation. [2-6] show a degraded NDR behavior after the initial electrical measurements when $x \geq 0.70$ in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaIn}$ double barrier RT structures. High aluminum content ($x \geq 0.70$) leads barrier designs leading to large lattice-mismatch at the hetero-interface. In order to improve material quality and to get reliable and reproducible NDR low aluminum content (20%) is employed. However, in this paper considering low aluminum content ($x=0.20$) in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier transmission coefficient is observed for varying barrier width and well width in presence and absence of applied field.

II. THEORY

Time-independent Hamiltonian eigenequation is given by [7]

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(z)}{dz^2} + V(z)\psi(z) = E\psi(z) \quad (1)$$

To describe the transfer matrix method the simple scenario in fig. 1 will be considered first. In region 1 the wave function is termed Ψ_1 and the potential is zero, in region 2 the wave function is termed Ψ_2 and the potential is V_0 and in region 3 the wave function is termed Ψ_3 and the potential is again zero. The solution to the Hamiltonian eigenvalue equation (1) in these three regions are

$$\psi_1 = A e^{ik_1 z} + B e^{-ik_1 z} \quad (2)$$

$$\psi_2 = C e^{ik_2 z} + D e^{-ik_2 z} \quad (3)$$

$$\psi_3 = F e^{ik_3 z} + G e^{-ik_3 z} \quad (4)$$

where, $k_i = \sqrt{2m(E - V_i)}$

V_0 is related to the band gap of AlGaIn by the relation below

$$V_0 = E_g(\text{AlGaIn}) - E_g(\text{GaIn}) - \Delta E_v \quad (5)$$

where, ΔE_v is valence band discontinuity.

Compositional and temperature dependence of the energy gap $E_g(x,T)$ of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys for the entire alloy range $0 \leq x \leq 1$ is given by [8]

$$E_g(x,T) = E_g(x,0) - \frac{\alpha(x)T^2}{\beta(x) + T^2} \quad (6)$$

where, $E_g(x,0)$ can be written in terms of low temperature band gaps of GaIn and AlN [8]

$$E_g(x,0) = (1-x)E_g(\text{GaIn}) + xE_g(\text{AlN}) - bx(1-x) \quad (7)$$

where, b is the bowing parameter.

α is an empirical constant and β is associated with Debye temperature. They can be written as [8]

$$\alpha(x) = (1-x)\alpha(\text{GaIn}) + x\alpha(\text{AlN}) - cx(1-x) \quad (8)$$

$$\beta(x) = (1-x)\beta(\text{GaIn}) + x\beta(\text{AlN}) - dx(1-x) \quad (9)$$

respectively, where, c and d are fitting parameters.

The wave function (2) and its derivative is required to be continuous at the discontinuity between adjacent regions, i.e. $z=0$ and $z=a$. Using the continuity conditions between region 1 and region 2 yields the two equations

$$\psi_1(0) = \psi_2(0) \quad (10)$$

$$\text{and } \frac{d\psi_1}{dz} \Big|_{z=0} = \frac{d\psi_2}{dz} \Big|_{z=0} \quad (11)$$

which gives the following restrictions on the coefficients

$$A + B = C + D \tag{12}$$

$$ik_1A - ik_1B = ik_2C - ik_2D \tag{13}$$

These conditions can be written in matrix form

$$\begin{pmatrix} 1 & 1 \\ ik_1 - ik_1 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik_2 - ik_2 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \tag{14}$$

(14) can be written as

$$\begin{pmatrix} A \\ B \end{pmatrix} = M_{12} \begin{pmatrix} C \\ D \end{pmatrix} \tag{15}$$

M_{12} is known as discontinuity matrix, it describes the propagation of the wave function across the boundary.

Using the transfer matrix technique (TMT) the final equation for a double barrier single well RTD can be formulated as

$$\begin{pmatrix} A \\ B \end{pmatrix} = M_{12} M_B M_{23} M_W M_{34} M_B M_{45} \begin{pmatrix} K \\ L \end{pmatrix} \tag{16}$$

or $\begin{pmatrix} A \\ B \end{pmatrix} = M_s \begin{pmatrix} K \\ L \end{pmatrix} \tag{17}$

where, (A,B) and (K,L) are coefficients of matrices for wave function profile of contact layers. M_s is known as system matrix.

(15) can be written as

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M_{11}M_{12} \\ M_{21}M_{22} \end{pmatrix} \begin{pmatrix} K \\ L \end{pmatrix} \tag{18}$$

Transmission coefficient can be formulated as the ratio between the flux incident from left side in the barrier and the transmitted flux in the right side, when no incident wave from the left.

$$f_{int} = |A|^2 \text{ and } f_{tran} = |K|^2$$

$$T(E) = \frac{f_{tran}}{f_{int}} = \frac{|K|^2}{|A|^2} = \frac{1}{|M_{11}|^2} \tag{19}$$

When electric field is applied the eigenvalue equation will be modified as

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(z)}{dz^2} + V(z)\psi(z) - q\zeta(z)z\psi(z) = E\psi(z) \tag{20}$$

Where $\zeta(z)$ is the electric field applied along the direction of confinement. Considering new coefficients (A,B) and (C,D) for contact layers, transmission coefficient can be obtained from the following expression

$$T(E) = \frac{|K|^2}{|A|^2} = \frac{1}{|M_{11}|^2} \tag{21}$$

III. RESULTS AND DISCUSSIONS

Using (1) to (4), (10) to (19) and with the help of fig. 1 transmission coefficient (Tc) of $Al_{0.2}Ga_{0.8}N/GaN$ double barrier single well and triple barrier double well RTDs under zero applied electric field are calculated. Transmission coefficient for varying composition of barrier is also calculated using (1) to (19) at $T=300K$. With the help of (1) to

(21) variation of Tc with applied electric field is calculated. Barrier width and well width are taken as 2 nm and 1 nm respectively unless otherwise stated. Here the value of V_0 for $Al_{0.2}Ga_{0.8}N$ barrier is considered as 0.42 eV [9] and the value of electron effective mass in hexagonal GaN is taken as $0.222m_0$ [10]. Fermi energy of GaN is considered as located about 0.08 eV above the conduction band minimum ($T=300K$) [11]. Fig. 2 shows the comparative analysis of transmission coefficient profile with electron energy for varying material composition in $Al_xGa_{1-x}N$ barrier. As x decreases from 1 to 0.2 bandgap of $Al_xGa_{1-x}N$ decreases and transmission probability of electrons from GaN contact layer through the barrier increases. Maximum tunneling probability occurs when mole fraction of Al in AlGaN barrier is 0.2. Variation of transmission coefficient with electron energy under zero applied bias for double barrier and triple barrier $Al_{0.2}Ga_{0.8}N/GaN$ RTDs are shown in fig. 3 and fig. 4 respectively. From the graphs it is seen that energy of the first quasi bound state is around 0.1 eV. No interesting details are seen above 0.52 eV where the transmission coefficient becomes very close to unity. This is because the barrier height was set to 0.42 eV and energy higher than this will produce transmission coefficients on the order of unity. Difference between the two plots is the splitting of the peaks into several closely spaced peaks when more barriers are added. In double barrier case peaks are located where true bound eigenstates would be located if the quantum well was infinitely wide. In triple barrier case it would thus seem like the presence of additional barriers results in additional bound eigenstates in the well. In fig. 5 the tunneling probability in a double barrier structure under an applied voltage between 0 V and 0.3 V is shown. This is due to the asymmetry of the barrier due to the applied field. When field is applied the barriers no longer have the same height for an electron of energy E. Comparing this graph to fig. 3 and fig. 4 the important result that Tc does not become unity when resonance occurs under applied voltage is apparent. Fig. 6 shows the variation of transmission coefficient with barrier width under zero applied bias. As the width increases tunneling probability of electron decreases for a fixed electron energy and Tc becomes unity for 1 nm $Al_{0.2}Ga_{0.8}N$ barrier width. Fig. 7 illustrates the effect of well width on Tc under zero applied field. As the well width increase lowest quantized energy level goes down as a result for small increase in electron energy transmission coefficient becomes nearly equal to 1. In fig. 8 a comparative analysis of transmission coefficient profile for different barrier width in presence of applied field is shown. Fig. 9 shows the effect of well width and applied field on Tc. Transmission coefficient is much less in both of these figures as electric field is applied.

TABLE I
Fitting parameters for bandgap of AlGaN in (6) at $T=300K$

Parameter	GaN	AlN
Bandgap	3.5 [8]	6.1 [8]
a (meV/K)	0.84 [12]	2.59 [12]
β (K)	789 [12]	2030 [12]
b (eV)	≈ 1 eV [8]	
c (meV/K)	2.15 [8]	
d (K)	1561 [8]	

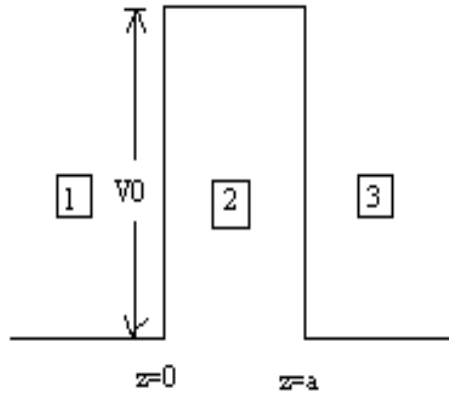


Figure 1. Tunneling through a single barrier

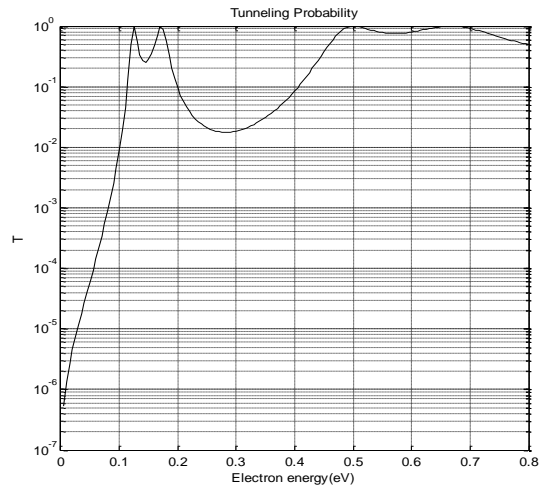


Figure 4. Transmission coefficient for triple barrier double well $Al_{0.2}Ga_{0.8}N/GaN$ RTD under zero applied electric field.

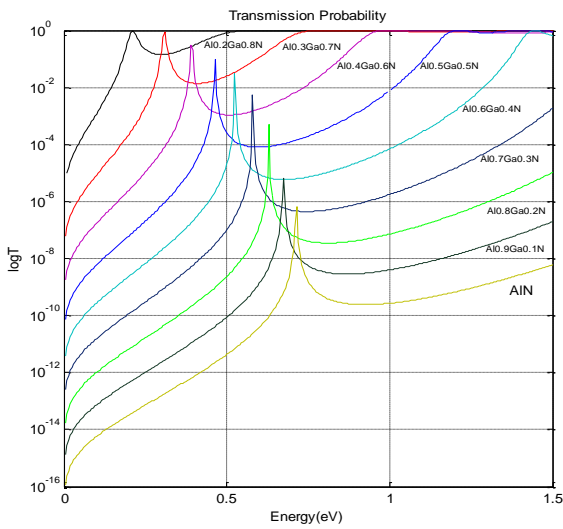


Figure 2. Comparative analysis of transmission coefficients profile for different material composition in AlGaIn barrier.

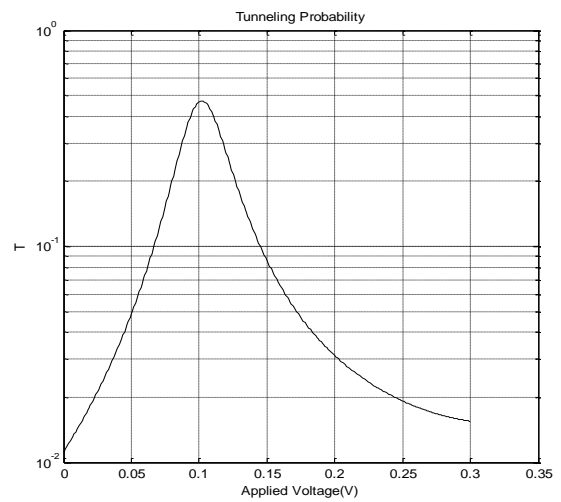


Figure 5. Tunneling probability under an applied voltage between 0V and 0.3V in a double barrier AlGaIn/GaN RTD

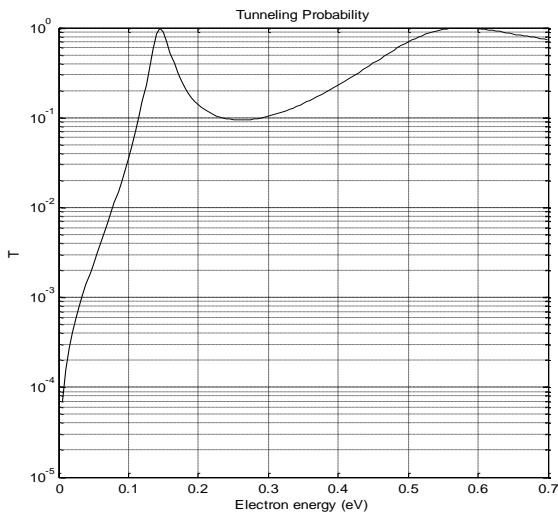


Figure 3. Transmission coefficient for double barrier single well $Al_{0.2}Ga_{0.8}N/GaN$ RTD under zero applied electric field.

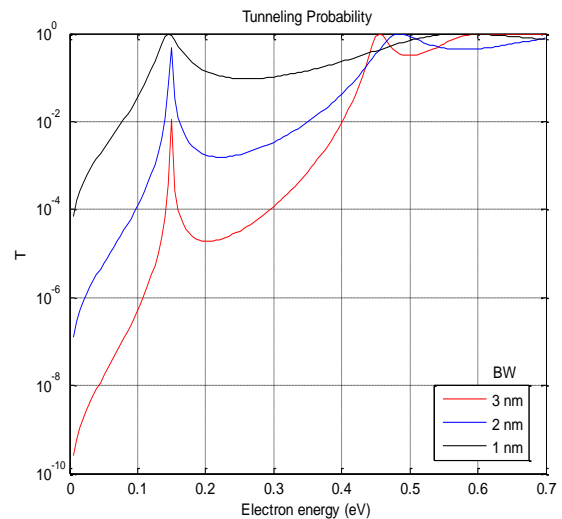


Fig. 6. Variation transmission coefficient with electron energy for different barrier width in absence of applied electric field.

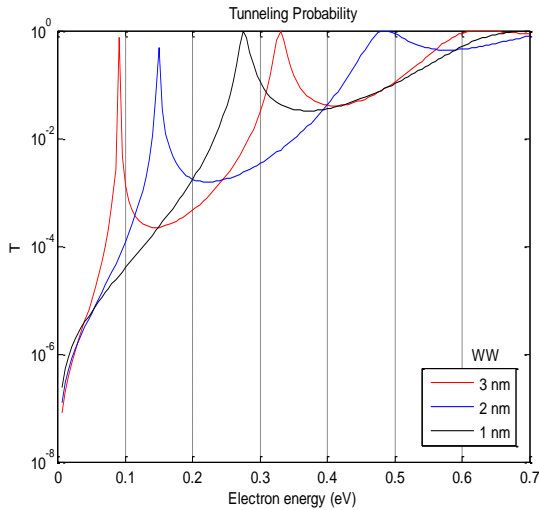


Figure 7. Comparative analysis of transmission coefficient profile for different well width in presence of applied electric field.

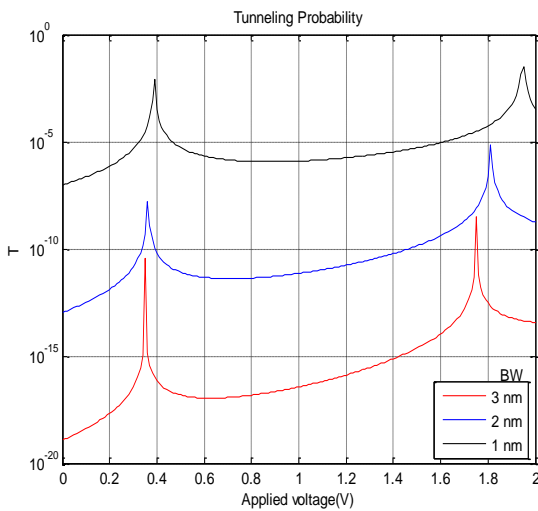


Figure 8. Effect of different barrier width and applied electric field on transmission coefficient of $Al_{0.2}Ga_{0.8}N/GaN$ RTD.

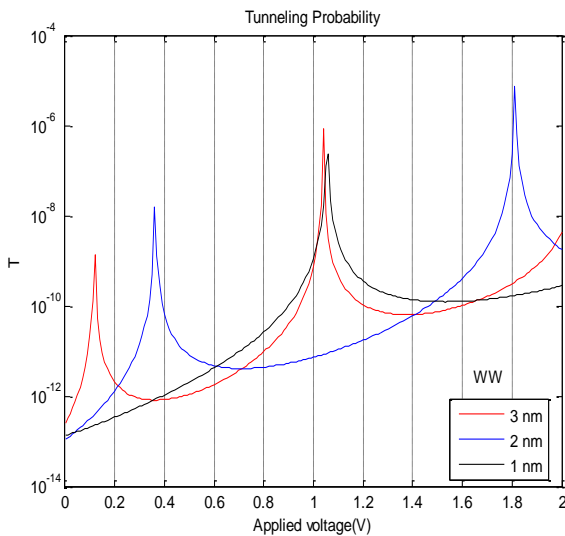


Figure 9. Variation of transmission coefficient with well width in presence of applied field.

IV. CONCLUSION

An analytical model for transmission coefficient (T_c) for AlGaIn/GaN RTDs is developed which takes into consideration well width, barrier width in presence and absence of applied field. It can be concluded that tunneling through symmetric double and triple barrier structures can reach T_c values of 1 when resonance occurs. It is also found that resonance peaks are split into several small peaks where the number of small peaks is generally equal to (number of barriers - 1). This study illustrates that in asymmetric barrier structures it is much harder to obtain T_c values of 1. It is concluded that absence of applied field is most favorable for AlGaIn/GaN RTDs and also thin barrier is preferred for maximum transmission coefficient.

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