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Calculating InN/GaN Transmission Coefficient from Single Barrier to Five Barriers with Propagation Matrix and Transfer Matrix Methods

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Abstract. In this study, the value of transmission coefficient on InN/GaN semiconductor from a single barrier to five barriers was determined by using the propagation matrix method and the transfer matrix method. This study aims to see the effect of adding a barrier to the number of resonance tunneling that occurs, to see the difference in transmission coefficient values which was obtained with the two methods, and to determine the effectiveness of the program execution process time from the propagation matrix and transfer matrix methods using Matlab programming. The results obtained indicated that the value of the transmission coefficient obtained from the two methods was the same. As the number of barriers increases, the number of resonance tunneling that occurs will increase. These two matrix methods had differences in terms of the effectiveness of the program execution process time and calculation process. The propagation matrix method was considered more effective than the transfer matrix method.

Keywords: *InN/GaN, Propagation Matrix Method, The Tunneling Effect, Transfer Matrix Method, Transmission Coefficient.*

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INTRODUCTION

The tunneling effect is a microscopic phenomenon in which a particle can break through the barrier potential so that the particle can move freely after penetrating the barrier. This quantum phenomenon was applied widely to semiconductors. The probability that a particle can penetrate the barrier is expressed in terms of the transmission coefficient (*T*) [1]. Many studies have been carried out on the analysis of the transmission coefficient of various semiconductor materials with various numbers and types of barriers through various calculation methods. Agustin *et al.* have analyzed the tunneling effect of InN from a single barrier to three barriers with the conventional analytic method [2]. Huda *et al.* have used the propagation matrix method to analyze the tunneling effect in four barriers of graphene [3]. The propagation matrix method has

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been used by Supriadi *et al*. to determine the transmission coefficient of three potential barriers which consisted of GaN, SiC, and GaAs [4]. Lolo has researched the tunneling resonance effect of $In_xGa_{1-x}As$/InP tensile strained with the method of transfer matrix [5].

The propagation matrix method is a method that is used to determine transmission and reflection coefficients by using matrix form. This method has the advantage that the process is the easiest to solve the problem of potential barriers in large quantities. This advantage appears because the analysis review area at any limit still returns to its initial state [6]. This method can be applied to various types of potential barrier shapes [7]. Another method called the transfer matrix method is a method that is used to solve second-order differential equations by using matrix form. It also can be used to determine transmission coefficient equations and can give efficient simulation that applied in many barriers cases because its implementation process was fast and its result was more accurate [8].

In this study, the equation of transmission coefficient on InN/GaN semiconductor from a single barrier to five barriers was determined by using two different numerical methods, namely the propagation matrix method and the transfer matrix method, and was simulated with Matlab programming. This study aimed to see the effect of adding a barrier to the number of resonance tunneling that occurs, to see the difference in transmission coefficient values which was obtained with the two methods, and to determine the effectiveness of the program execution process time from the propagation matrix and transfer matrix methods using Matlab programming.

RESEARCH METHODS

In this study, InN/GaN heterostructure was used as the barrier potential with the barrier's strength of 2.22 eV. This value was taken by the value of the conduction band offset of the InN/GaN heterostructure [9]. GaN was considered a barrier and InN was considered a well or a gap between barriers. The distance between barriers was taken from InN's lattice constant equal to 0.3533 nm and the width of barrier potential was taken from GaN's lattice constant equal to 0.3189 nm [10]. Effective electron mass inside and outside the barrier were 0.22 $m_0$and 0.12 m_0 respectively [11]. The electron energy was smaller than barrier potential ($E < V$) with variation values from 0.003 eV to 2.0 eV. The simulation process was carried out using Matlab programming. The model of the InN/GaN barrier potential structure was shown in Fig. 1.

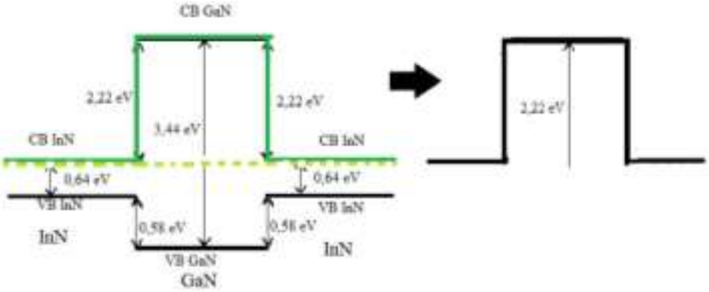


FIGURE 1. The model of an InN/GaN barrier potential structure.

RESULTS AND DISCUSSIONS

Transmission Coefficient Equation with Propagation Matrix Method

A single barrier potential was rectangular with a potential high of V_0 and a barrier width of L was described such as Fig. 2. On a heterostructure semiconductor, effective electron masses were different both inside and outside of the barrier. Effective electron mass inside the barrier was expressed by m_b. Whereas effective electron mass outside the barrier was expressed by m_w.

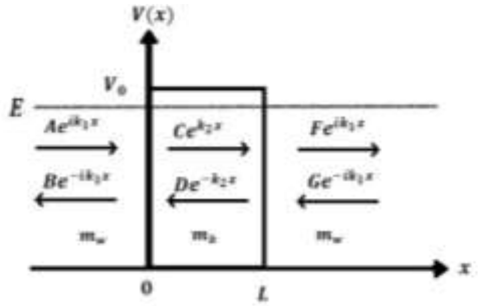


FIGURE 2. The Heterostructure Single Barrier Potential model ($m_w \neq m_b$)

The wave function equations on each area:

$$\psi_I = Ae^{ik_1x} + Be^{-ik_1x} \tag{1}$$

$$\psi_{II} = Ce^{k_2x} + De^{-k_2x} \tag{2}$$

$$\psi_{III} = Fe^{ik_1x} + Ge^{-ik_1x} \tag{3}$$

where $k_1 = \frac{(2m_wE)^{1/2}}{\hbar}$ and $k_2 = \frac{(2m_b(V_0-E))^{1/2}}{\hbar}$.

At the boundary *x=0*, the continuity condition was applied.

$$\psi_I|_{x=0} = \psi_{II}|_{x=0} \tag{4}$$

$$A + B = C + D \tag{5}$$

$$\frac{1}{m_w}\frac{d\psi_I}{dx}\bigg|_{x=0} = \frac{1}{m_b}\frac{d\psi_{II}}{dx}\bigg|_{x=0} \tag{6}$$

$$\frac{ik_1(A-B)}{m_w} = \frac{k_2(C-D)}{m_b} \tag{7}$$

Eq. (5) and Eq. (7) were converted in matrix form to

$$\begin{bmatrix} A \\ B \end{bmatrix} = \boldsymbol{P_{step-up}} \begin{bmatrix} C \\ D \end{bmatrix} \tag{8}$$

$$\boldsymbol{P_{step-up}} = \frac{1}{2}\begin{bmatrix} 1 + \frac{m_wk_2}{m_bik_1} & 1 - \frac{m_wk_2}{m_bik_1} \\ 1 - \frac{m_wk_2}{m_bik_1} & 1 + \frac{m_wk_2}{m_bik_1} \end{bmatrix} \tag{9}$$

Determining the propagation matrix for the propagation of wave function between $x = 0$ and $x = L$ with a barrier width of L ($\boldsymbol{P_{free}}$). The wave functions equation in this boundary was formed by Bloch's Theorem.

$$Ce^{k_2L} = F \tag{10}$$

$$De^{-k_2L} = G \tag{11}$$

Eq. (10) and Eq. (11) were converted in matrix form to

$$\begin{bmatrix} C \\ D \end{bmatrix} = \boldsymbol{P_{free}} \begin{bmatrix} F \\ G \end{bmatrix} \tag{12}$$

$$\boldsymbol{P_{free}} = \begin{bmatrix} e^{-k_2 L} & 0 \\ 0 & e^{k_2 L} \end{bmatrix} \tag{13}$$

Determining the propagation matrix on boundary $x = L$ ($\boldsymbol{P_{step-down}}$). This barrier consisted of step-up and step-down. Therefore, to analyze at $x = L$ boundary, it can be viewed back as the initial review when we determined $\boldsymbol{P_{step-up}}$ matrix at $x = 0$ before. $\boldsymbol{P_{step-down}}$ matrix could be obtain easily by replaced $\frac{m_w k_2}{m_b i k_1}$ became $\frac{m_b i k_1}{m_w k_2}$ in $\boldsymbol{P_{step-up}}$ matrix.

$$\boldsymbol{P_{step-down}} = \frac{1}{2} \begin{bmatrix} 1 + \dfrac{m_b i k_1}{m_w k_2} & 1 - \dfrac{m_b i k_1}{m_w k_2} \\ 1 - \dfrac{m_b i k_1}{m_w k_2} & 1 + \dfrac{m_b i k_1}{m_w k_2} \end{bmatrix} \tag{14}$$

Therefore, the propagation matrix of one unit barrier ($\boldsymbol{P_j}$) was

$$\boldsymbol{P_j} = \boldsymbol{P_{step-up}} \boldsymbol{P_{free}} \boldsymbol{P_{step-down}} \tag{15}$$

where $\boldsymbol{P_j}$ was 2×2 matrix form.

$$\boldsymbol{P_j} = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} \tag{16}$$

Numerically, the value of transmission coefficient could be determined by the equation

$$T = \left| \frac{1}{p_{11}} \right|^2 = \left[1 + \frac{\left({k_1}^2 {m_b}^2 + {k_2}^2 {m_w}^2 \right)^2}{4 {k_1}^2 {k_2}^2 {m_b}^2 {m_w}^2} \sinh^2(k_2 L) \right]^{-1} \tag{17}$$

This equation was the transmission coefficient equation of single barrier potential case. For many barriers, total propagation matrix equation ($\boldsymbol{P}$) could be calculated by

$$\boldsymbol{P} = \boldsymbol{P_1 P_2} \dots\dots = \prod_{\boldsymbol{j=1}}^{\boldsymbol{j=N}} \boldsymbol{P_j} \tag{18}$$

where $\boldsymbol{P_j} = \boldsymbol{P_{step-up\ j}} \boldsymbol{P_{free\,j}} \boldsymbol{P_{step-down\,j}}$; $j = 1,2,3,4,5$.

Transmission Coefficient Equation with Transfer Matrix Method

With the same barrier model as in Fig. 2, the wave function of each region can be determined and the boundary conditions of each boundary plane can be imposed. Then, the equations that have been obtained can be made into a matrix form.

The matrix equation at *x=0* boundary was

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \dfrac{m_w k_2}{m_b i k_1} & -\dfrac{m_w k_2}{m_b i k_1} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}$$

$$M_1 \begin{bmatrix} A \\ B \end{bmatrix} = M_2 \begin{bmatrix} C \\ D \end{bmatrix} \tag{19}$$

The matrix equation at *x=L* boundary was

$$\begin{bmatrix} e^{k_2L} & e^{-k_2L} \\ e^{k_2L} & -e^{-k_2L} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} e^{ik_1L} & e^{-ik_1L} \\ \frac{m_b ik_1}{m_w k_2} e^{ik_1L} & -\frac{m_b ik_1}{m_w k_2} e^{-ik_1L} \end{bmatrix} \begin{bmatrix} F \\ G \end{bmatrix}$$

$$M_3 \begin{bmatrix} C \\ D \end{bmatrix} = M_4 \begin{bmatrix} F \\ G \end{bmatrix} \tag{20}$$

Total transfer matrix equation of single barrier was

$$\begin{pmatrix} A \\ B \end{pmatrix} = M_1^{-1} M_2 M_3^{-1} M_4 \begin{pmatrix} F \\ G \end{pmatrix}$$

$$= M \begin{pmatrix} F \\ G \end{pmatrix} \tag{21}$$

Where matrix M was 2×2 matrix form.

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \tag{22}$$

Numerically, the value of transmission coefficient could be determined by the equation

$$T = \left| \frac{1}{M_{11}} \right|^2$$

$$= \left[1 + \frac{((m_b k_1)^2 + (m_w k_2)^2)^2}{4 {k_1}^2 {k_2}^2 {m_b}^2 {m_w}^2} \sinh^2(k_2 L) \right]^{-1} \tag{23}$$

In the same way, the transmission coefficient equation for two, three, four, and five barriers can be determined by extending the total transfer matrix equation. We directly show the total transfer matrix for five barriers because one just need to simplify this equation for the less barriers cases. This equation is denoted by

$$\begin{pmatrix} A \\ B \end{pmatrix} = M_1^{-1} M_2 M_3^{-1} M_4 \ldots\ M_{17}^{-1} M_{18} M_{19}^{-1} M_{20} \begin{pmatrix} Y \\ Z \end{pmatrix} \tag{24}$$

where the model of five barriers was described such as Fig. 3.

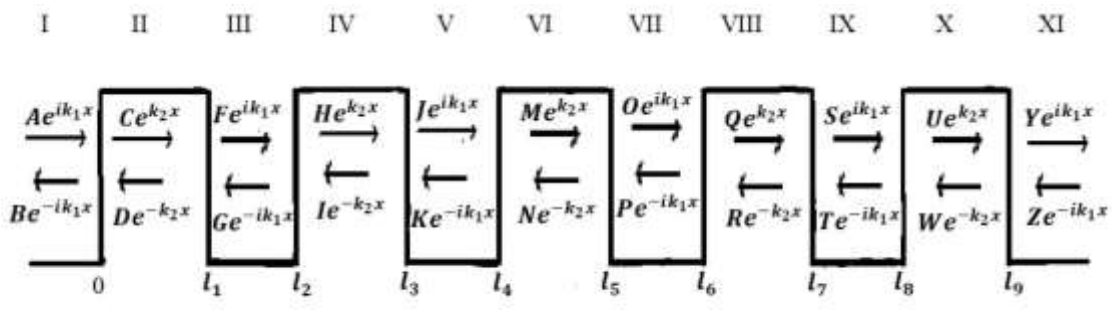


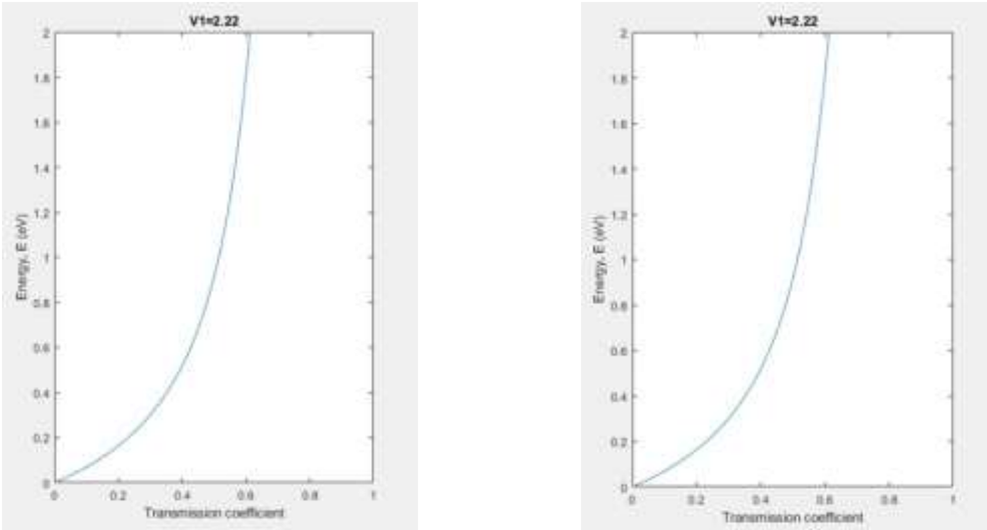
FIGURE 3. The Heterostructure Five Barriers Potential model ($m_w \neq m_b$)

Transmission Coefficient Simulation Results

Simulation of the tunneling effect was carried out on each multiple barriers using the propagation matrix and transfer matrix methods to obtain the transmission coefficient value. In this case, electron was coming from the left to the right of the barrier.

Simulation Result on Single Barrier Potential

The resulting transmission coefficient value on a single barrier, using the two different methods, was the same. The transmission coefficient increased exponentially up to 0.613 at an electron energy of 2.00 eV as shown in Fig. 4.

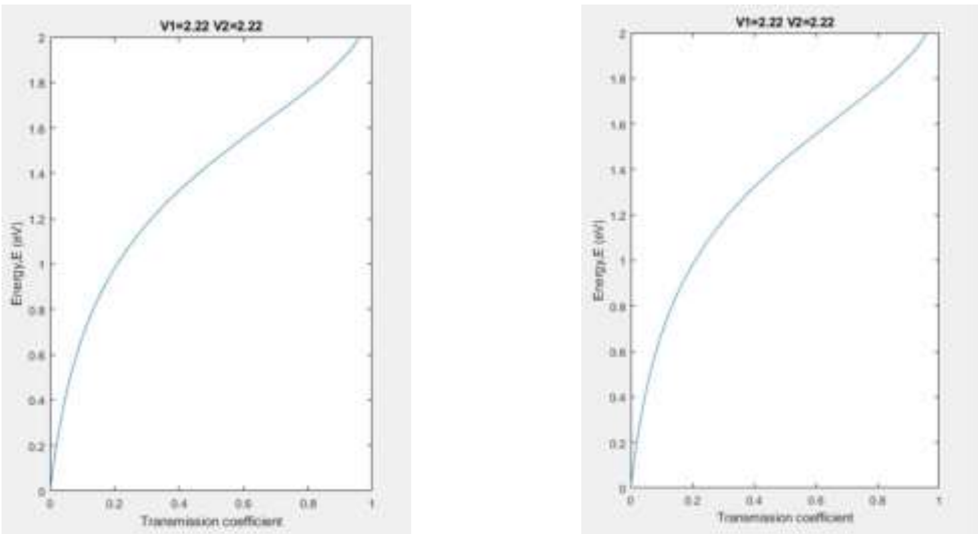


(a) (b)

FIGURE 4. Graph of the relationship between electron energy and transmission coefficient on a single barrier structure with (a) propagation matrix method and (b) transfer matrix method

Simulation Result on Two Barriers Potential

The resulting transmission coefficient value on two barriers, using the two different methods, was the same. The Transmission coefficient increased up to the maximum value of 0.961 at an electron energy of 2.00 eV as shown in Fig. 5.

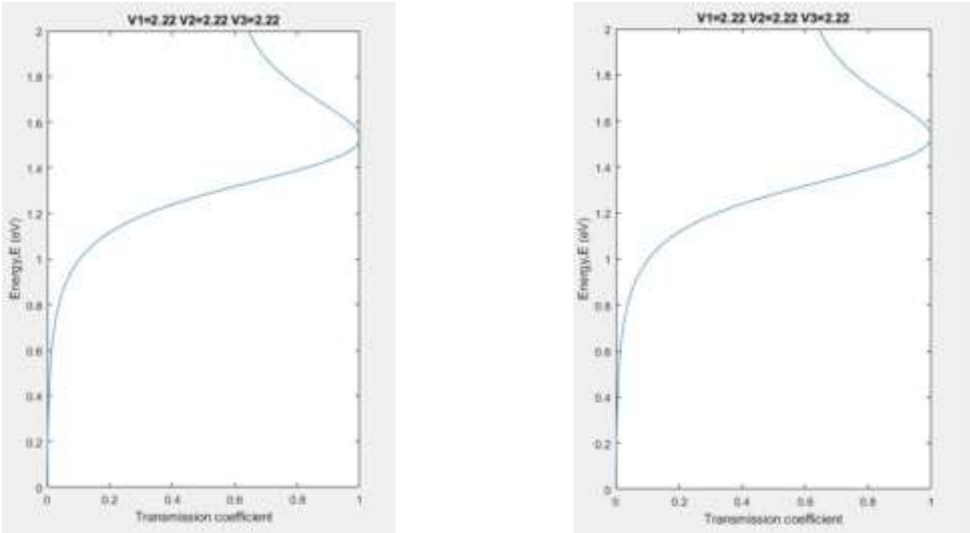


(a) (b)

FIGURE 5. Graph of the relationship between electron energy and transmission coefficient on two barriers structure with (a) propagation matrix method and (b) transfer matrix method

Simulation Result on Three Barriers Potential

The resulting transmission coefficient value on three barriers, using the two different methods, was the same. The transmission coefficient increased to the maximum value of 1 at an electron energy of 1.532 eV and it decreased to the value of 0.644 at an electron energy of 2.00 eV. The existence of a transmission coefficient value of 1, in this case, indicated that there was one resonance tunneling at an electron energy value of 1.532 eV as shown in Fig. 6.



(a) (b)

FIGURE 6. Graph of the relationship between electron energy and transmission coefficient on three barriers structure with (a) propagation matrix method and (b) transfer matrix method

Simulation Result on Four Barriers Potential

The resulting transmission coefficient value on four barriers, using the two different methods, was the same. The transmission coefficient increased to the maximum value of 1 at an electron energy of 1.300 eV and it decreased to the value of 0.547 at an electron energy of 1.600 eV. Then, the transmission coefficient value rose to the value of 0.867 at an electron energy of 2.00 eV as shown in Fig. 7. This result indicated that there was one resonance tunneling at an electron energy value of 1.300 eV and the transmission coefficient value fluctuated with variations of electron energy.

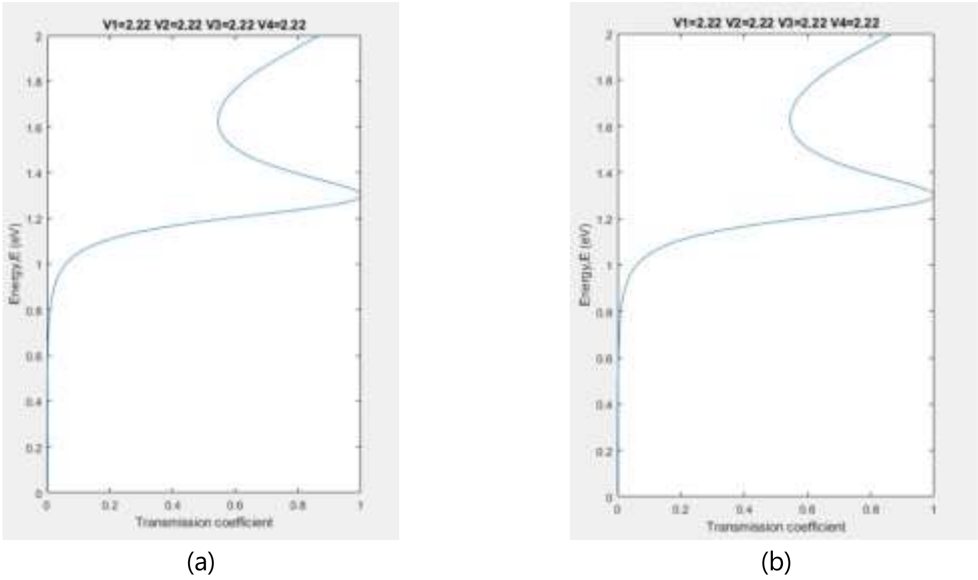


FIGURE 7. Graph of the relationship between electron energy and transmission coefficient on four barriers structure with (a) propagation matrix method and (b) transfer matrix method

Simulation Result on Five Barriers Potential

The resulting transmission coefficient value on five barriers, using the two different methods, was the same as shown in Fig. 8.

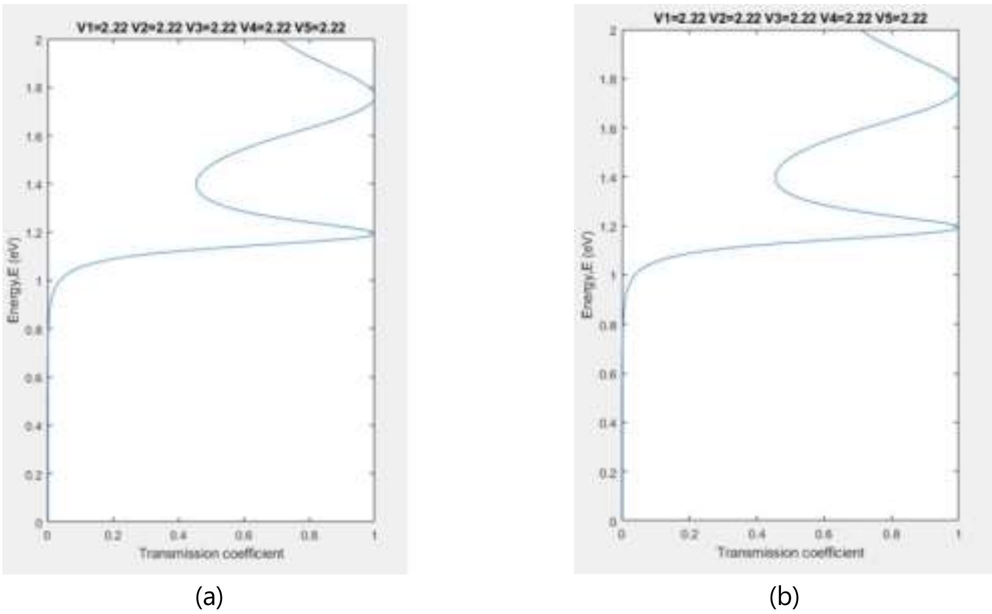


FIGURE 8. Graph of the relationship between electron energy and transmission coefficient on five barriers structure with (a) propagation matrix method and (b) transfer matrix method

The transmission coefficient increased until it reached a maximum value of 1 at the electron energy value of 1.194 eV. After reached this value, transmission coefficient decreased to the value of 0.454 at an electron energy of 1.400 eV and grew up back to the maximum value of 1 at an electron energy of 1.762 eV before down to the value of

0.707 at an electron energy of 2.00 eV This result indicated that, in this case, resonance tunneling occurred twice at an electron energy value of 1.194 eV and 1.762 eV.

According to these results, it can be seen that transmission coefficient value that obtained from propagation matrix method and transfer matrix method had the same value in each electron energy variation. So that there was no difference in the value of the transmission coefficient between the two methods. Although there was no difference in the value of the transmission coefficient, these two methods had differences based on the effectiveness of the program execution process time and the implementation process in determining matrix equations.

Table 1. Average Program Execution Process Time from Single Barrier to Five barriers by using Propagation Matrix and Transfer Matrix Method

Number of Barriers	**Average Program Execution Process Time (seconds)**	
	Propagation Matrix Method	**Transfer Matrix Method**
One	±1.0	±34.6
Two	±1.0	±34.2
Three	±1.0	±34.2
Four	±1.0	±35.2
Five	±1.0	±35.0
Average	**±1.0**	**±34.64**

Based on Table 1. It can be seen that program execution process with propagation matrix method took approximately one second. While the transfer matrix method required approximately 34.64 seconds. It can be shown that the propagation matrix method was considered to be more effectively applied in computational simulations than the transfer matrix method.

The addition of the number of barriers affected the amount of resonance tunneling that occurs in InN/GaN semiconductors. The more we add the barriers, the more resonant tunneling will occur at certain energy values. The value of the transmission coefficient fluctuated with variations in electron energy as in the results of previous studies [2].

CONCLUSIONS

The values of the InN/GaN transmission coefficient from a single barrier to five barriers have been obtained by using the propagation matrix method and the transfer matrix method. The more we add the barriers, the more resonant tunneling will occur at certain energy values. There was no difference in transmission coefficient values which was obtained with the two methods. These two matrix methods have differences in terms of the effectiveness of the program execution process time and calculation process. The propagation matrix method was considered more effective than the transfer matrix method.

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