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Transmittance on combinatorial structures of triple potential barriers

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Abstract. Semiconductor materials used as potential barriers in the study are GaAs, GaSb, and AlAs. These materials will be arranged in certain combinations to form triple potential barrier structures and the effect of combinations will be analysed against transmission coefficient values. In this study, the maximum energy of the electron is 1 eV and the matrix propagation method is used where the effect of the combinations structure on transmission coefficient values is numerically analysed using a computational program. The results showed that the structuring potential barrier affects the value of the transmission coefficient. In the uniform barriers arrangements, the value of the transmission coefficient decreases with increasing potential barrier energy. Whereas in the arrangement of different barrier combinations, two opposing combination arrangements have the same transmission coefficient values. Thus, from six combination arrangements, there are three kinds of transmission coefficient values. The maximum transmission coefficient value is 1.000 in the triple potential barrier of GaSb at 0.49 eV. Research on the tunnel effect contributed to the development of electronic and optoelectronic devices such as transistors and lasers.

1. Introduction

In the 19th century, new phenomena related to the concept of modern physics began to appear. New phenomena are related to physical objects of microscopic size such as atoms and particles which cannot be explained by the concept of classical physics. This is what causes scientists to develop new theories that can explain the physical behavior of particles and atoms. The branch of Physics that can answer these problems is called quantum mechanics.

One of the interesting phenomena in quantum mechanics is the tunneling effect. Tunneling effect is a state where quantum electrons can pass through the potential barrier even though their energy is less than the potential energy of the barrier. Tunneling effect allows particles with less energy to pass through a potential barrier and given the opportunity for transmission. The transmission coefficient is the probability that a particle can break through a potential barrier [4]. The tunneling effect is widely applied in everyday life, including in the development of nano-scale electronic devices. The sophisticated electronic equipment used in today's technology cannot be separated from the use of transistors. Electronic devices such as transistors and ICs use semiconductor materials because these materials have a barrier potential.

A semiconductor is a material that has electrical conductivity between the insulator and the conductor [11]. In general, the basic components of active electronics such as diodes, transistors, and ICs (Integrated Circuits) are made of semiconductor materials. In semiconductor materials there is an empty area between the valence band and the conduction band which is called the bandgap energy. Every



semiconductor material has a different energy gap at a certain temperature [5]. GaAs is a material with great potential for electronic and optoelectronic device applications because of its high electron mobility. GaAs is typically used for laser diodes and high-speed transistors. GaAs has an energy band gap structure with a direct transition (direct band gap) of 1.424 eV with a width of 0.565 nm [8]. GaSb is an alloy III-V semiconductor material that has a direct band gap with an energy band gap of 0.721 eV at room temperature [7] with a width of 0.610 nm [10]. Antimony-based alloy semiconductors have relatively high carrier mobility properties. With these properties, this material is interesting to be applied in electronic and optoelectronic devices such as lasers, infrared detectors, magnetic sensors and high-speed switching devices [3]. AlAs is a III-V alloy semiconductor material which is widely applied to optoelectronic devices such as laser diodes. AlAs has a fairly large energy band gap of about 2.95 eV [10] with a width of 0.566 nm [2]. With a lattice constant similar to GaAs, AlAs has a small induced voltage which allows high mobility of high-performance electrons, so that AlAs can also be applied to HEMT (High Electron Mobility Transistor) transistors [1].

In this study, GaAs, GaSb, and AlAs semiconductors were used. GaAs was chosen because GaAs is a potential material for electronic device applications with an energy band gap of 1.424 eV [8]. GaSb material has a high enough mobility which can produce high-speed devices with an energy band of 0.721 eV [7]. In addition, AlAs material is widely applied in diode lasers because AlAs has a large energy band gap of 2.95 eV [10]. Apart from being characterized by the presence of barrier potential energy, semiconductor materials also have the characteristics of the width of the barrier they have. GaSb has a barrier width of 0.610 nm [10], GaAs has a barrier width of 0.565 nm [8], and AlAs has a similar barrier width to GaAs of 0.566 nm [2]. GaAs, GaSb, and AlAs materials will be arranged in certain combinations to form a triple potential barrier structure and then analyzed the effect of the combination on the value of the transmission coefficient. In this study the matrix propagation method is used to analyze the transmission coefficient. The matrix propagation method is the spread or transmission of a wave using a matrix [6]. The matrix propagation method is easier to understand and the operation is very simple, where the effect of the combination arrangement on the transmission coefficient is analyzed numerically using a computer program.

2. Method

The tunneling effect is a phenomenon in quantum physics when a particle with energy E breaks through the potential barrier V ($V > E$). In this study, the semiconductor materials used as a barrier are Gallium Arsenide (GaAs), Gallium Antimonide (GaSb), and Aluminum Arsenide (AlAs), each of which has a potential energy of 0.721 eV, 1.424 eV, and 2.95 eV. The electron particle is passed through the barrier potential with the energy regulated in the range $0 \leq E \leq 1$ eV. The potential barriers to each other are arranged with a gap width of 1 nm.

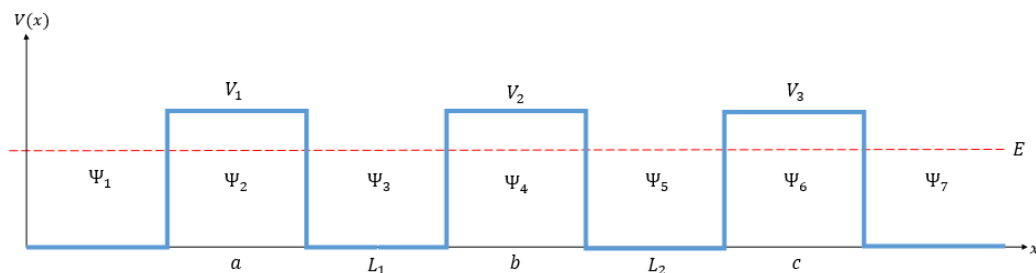


Figure 1. Triple barrier potential model

The mathematical solution for a particle with momentum p must be a wave function with $\lambda = h/p$ [9]. Where $p = \hbar k$, the kinetic energy of the free particle with de Broglie wavelength can be formulated as follows:

$$K = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \quad (1)$$

Figure 1 shows the triple barrier potential model with barrier widths a, b , and c . Ψ represents the wave function of the particle with the wave number k which has an energy of E . It can be seen that in the region 1 or $x < 0$ the particle acts as a free particle because the particle is not affected by any force or $V(x) = 0$. So that the particle has a wave number $k_1 = \frac{1}{\hbar}\sqrt{2mE}$. The free particle, then moves from left to right, when the particle enters the $0 \leq x \leq a$ region, the particle encounters a potential of $V = V_0$, so the particle has $k_2 = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$. Because $V_0 > E$, then $k_2 = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$ can be written as $k_2 = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$ or $k_2 = iq$, where $q = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$. When the particle successfully breaks through to $x > a$, the particle returns to a free particle with $V = 0$, so the particle has $k_3 = k_1 = \frac{1}{\hbar}\sqrt{2mE}$. The wave functions associated with these wave numbers are

$$\Psi_1(x) = \frac{A}{\sqrt{k_1}}e^{ik_1x} + \frac{B}{\sqrt{k_1}}e^{-ik_1x} \quad (2)$$

$$\Psi_2(x) = \frac{C}{\sqrt{k_2}}e^{k_2x} + \frac{D}{\sqrt{k_2}}e^{-k_2x} \quad (3)$$

$$\Psi_3(x) = \frac{F}{\sqrt{k_1}}e^{ik_1x} + \frac{G}{\sqrt{k_1}}e^{-ik_1x} \quad (4)$$

$$\Psi_4(x) = \frac{H}{\sqrt{k_3}}e^{k_3x} + \frac{I}{\sqrt{k_3}}e^{-k_3x} \quad (5)$$

$$\Psi_5(x) = \frac{J}{\sqrt{k_1}}e^{ik_1x} + \frac{L}{\sqrt{k_1}}e^{-ik_1x} \quad (6)$$

$$\Psi_6(x) = \frac{M}{\sqrt{k_4}}e^{k_4x} + \frac{N}{\sqrt{k_4}}e^{-k_4x} \quad (7)$$

$$\Psi_7(x) = \frac{O}{\sqrt{k_1}}e^{ik_1x} + \frac{Q}{\sqrt{k_1}}e^{-ik_1x} \quad (8)$$

where $A, B, C, D, F, G, H, I, J, L, M, N, O$, and Q are constants.

First, we examine the wave functions Ψ_1 and Ψ_2 which are bound by boundary conditions so that the wave function must meet the continuity requirements, namely

$$\Psi_1|_{step} = \Psi_2|_{step}$$

and

$$\left. \frac{d\Psi_1}{dx} \right|_{step} = \left. \frac{d\Psi_2}{dx} \right|_{step}$$

by applying the boundary conditions obtained

$$\frac{A}{\sqrt{k_1}} + \frac{B}{\sqrt{k_1}} = \frac{C}{\sqrt{k_2}} + \frac{D}{\sqrt{k_2}} \quad (9)$$

and

$$\frac{A}{\sqrt{k_1}} - \frac{B}{\sqrt{k_1}} = \frac{k_2}{ik_1} \frac{C}{\sqrt{k_2}} - \frac{k_2}{ik_1} \frac{D}{\sqrt{k_2}} \quad (10)$$

Equations (9) and (10) can be rewritten in matrix form

$$\frac{1}{\sqrt{k_1}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \frac{1}{\sqrt{k_2}} \begin{bmatrix} 1 & 1 \\ \frac{k_2}{ik_1} & -\frac{k_2}{ik_1} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} \quad (11)$$

To eliminate the 2×2 matrix on the left must be multiplied by the inverse of the matrix. So that equation (11) can be rewritten with

$$\begin{bmatrix} A \\ B \end{bmatrix} = \frac{1}{2\sqrt{k_1k_2}} \begin{bmatrix} k_1 - ik_2 & k_1 + ik_2 \\ k_1 + ik_2 & k_1 - ik_2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} \quad (12)$$

From equation (12) it can be seen that the propagation for the potential step up 1 is

$$\hat{p}_{step\ up\ 1} = \frac{1}{2\sqrt{k_1 k_2}} \begin{bmatrix} k_1 - ik_2 & k_1 + ik_2 \\ k_1 + ik_2 & k_1 - ik_2 \end{bmatrix} \quad (13)$$

The propagation in the $0 \leq x \leq a$ region can be calculated by:

$$\begin{aligned} \Psi C e^{k_2 a} &= \Psi F \\ \Psi D e^{-k_2 a} &= \Psi G \end{aligned}$$

if written in the matrix yet then

$$\begin{aligned} \begin{bmatrix} e^{k_2 a} & 0 \\ 0 & e^{-k_2 a} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} &= \begin{bmatrix} F \\ G \end{bmatrix} \\ \begin{bmatrix} C \\ D \end{bmatrix} &= \begin{bmatrix} e^{-k_2 a} & 0 \\ 0 & e^{k_2 a} \end{bmatrix} \begin{bmatrix} F \\ G \end{bmatrix} \end{aligned} \quad (14)$$

So the propagation across the potential barrier is

$$\hat{p}_{free\ 1} = \begin{bmatrix} e^{-k_2 a} & 0 \\ 0 & e^{k_2 a} \end{bmatrix} \quad (15)$$

In the same way when calculating $\hat{p}_{step\ up\ 1}$, $\hat{p}_{step\ down\ 1}$ can be calculated by applying the continuity condition to the potential boundary between Ψ_2 dan Ψ_3 obtained:

$$\hat{p}_{step\ down\ 1} = \frac{1}{2\sqrt{k_1 k_2}} \begin{bmatrix} k_2 + ik_1 & k_2 - ik_1 \\ k_2 - ik_1 & k_2 + ik_1 \end{bmatrix} \quad (16)$$

The total propagation of the first potential barrier is the product of the propagation step up 1, the propagation of the area between the step up potential 1 and the propagation step down 1.

$$\begin{aligned} \hat{P}_1 &= \hat{p}_{step\ up\ 1} \cdot \hat{p}_{free\ 1} \cdot \hat{p}_{step\ down\ 1} \\ \hat{P}_1 &= \frac{1}{2\sqrt{k_1 k_2}} \begin{bmatrix} k_1 - ik_2 & k_1 + ik_2 \\ k_1 + ik_2 & k_1 - ik_2 \end{bmatrix} \begin{bmatrix} e^{-k_2 a} & 0 \\ 0 & e^{k_2 a} \end{bmatrix} \frac{1}{2\sqrt{k_1 k_2}} \begin{bmatrix} k_2 + ik_1 & k_2 - ik_1 \\ k_2 - ik_1 & k_2 + ik_1 \end{bmatrix} \end{aligned} \quad (17)$$

$$\hat{P}_1 = \frac{1}{4k_1 k_2} \begin{bmatrix} (k_1 - ik_2)e^{-k_2 a} & (k_1 + ik_2)e^{k_2 a} \\ (k_1 + ik_2)e^{-k_2 a} & (k_1 - ik_2)e^{k_2 a} \end{bmatrix} \begin{bmatrix} k_2 + ik_1 & k_2 - ik_1 \\ k_2 - ik_1 & k_2 + ik_1 \end{bmatrix} \quad (18)$$

Meanwhile, the propagation of the triple potential barrier consists of 3 propagation steps up ($\hat{p}_{step\ up\ 1}$, $\hat{p}_{step\ up\ 2}$ and $\hat{p}_{step\ up\ 3}$), 3 propagations on the potential barrier ($\hat{p}_{free\ 1}$, $\hat{p}_{free\ 3}$ and $\hat{p}_{free\ 5}$), 2 propagations in the gap between the step up potential ($\hat{p}_{free\ 2}$ and $\hat{p}_{free\ 4}$) and 3 step down propagation ($\hat{p}_{step\ down\ 1}$, $\hat{p}_{step\ down\ 2}$ and $\hat{p}_{step\ down\ 3}$). The propagation on the triple barrier is stated:

$$\hat{P} = \hat{P}_1 \cdot \hat{P}_2 \cdot \hat{P}_3 \quad (19)$$

where

$$\begin{aligned} \hat{P}_1 &= \hat{p}_{step\ up\ 1} \cdot \hat{p}_{free\ 1} \cdot \hat{p}_{step\ down\ 1} \\ \hat{P}_2 &= \hat{p}_{free\ 2} \cdot \hat{p}_{step\ up\ 2} \cdot \hat{p}_{free\ 3} \cdot \hat{p}_{step\ down\ 2} \\ \hat{P}_3 &= \hat{p}_{free\ 4} \cdot \hat{p}_{step\ up\ 3} \cdot \hat{p}_{free\ 5} \cdot \hat{p}_{step\ down\ 3} \end{aligned}$$

so

$$\hat{P} = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix}$$

and the transmission coefficient in the matrix propagation method is expressed by:

$$T_3 = \frac{1}{|P_{11}|^2} \quad (20)$$

The triple barrier potential model consists of two structures, the first with the same three materials and the second, the combination arrangement of GaAs, GaSb, and AlAs. So that there are 6 combination arrangements. The transmission coefficient is obtained by analytical and numerical calculations. The analytical calculation is in the form of calculating the transmission coefficient of free particles when experiencing a breakthrough effect using the matrix propagation method. Numerical calculations are carried out by applying the matrix propagation method to the Matlab2018a software.

3. Result and Discussion

3.1. Analytic analysis

The tunneling effect is a phenomenon when particles break through a potential barrier that classical physics cannot do. The electrons are represented by the wave function Ψ in each region. The electrons moving from the left towards the first barrier have a momentum of $\sqrt{2mE}$. However, when the electron is in the potential region of V_j , it will be inhibited until it has a momentum of $\sqrt{2m(V_j - E)}$ where j is the sequence of barrier potentials ($j = 1, 2, 3$). After breaking through the potential barrier, the electron will accelerate until it has momentum $\sqrt{2mE}$ in the region $V = 0$ eV. The wave function representing electrons has a different shape in the region $V = 0$ and $V = V_j$. In the region $V = 0$, the wave function in the complex exponential form with value k_1x is imaginary (i). However, when the electron is in the potential region $V = V_j$, the wave function is exponential with the value k_jx is real where $j = 2, 3, 4$. This happens because in the $V = 0$ regions, electrons have material properties.

When electrons break through the barrier, according to de Broglie's postulate, the properties of the particles change to wave properties. Based on the research results, the transmission coefficient value of the breakthrough effect that occurs when the electrons break through the triple potential barrier GaSb, GaAs, and AlAs is obtained by using the matrix propagation method, analytically, it is obtained the equation of the transmission coefficient on the triple potential barrier, namely

$$T_3 = \frac{T_1 |t_2|^2 |t_3|^2}{\left| 1 - (\alpha + i\beta) e^{ik_1(L_1+L_2)} - \frac{r_1 r_3 t_2}{t_2^*} e^{i2k_1(L_1+L_2)} \right|^2} \quad (21)$$

where T_1 is the value of the transmission coefficient on the barrier 1, t_j (with $j = 2$ and 3) are the values of the transmission coefficient on the barrier j and r_j (with $j = 1, 2$, and 3) are the values of reflection coefficient on the barrier j .

3.2. Numeric analysis

This research examines the effect of the potential barrier arrangement on the transmission coefficient. The potential barrier arrangement is divided into two, namely an arrangement with a uniform barrier type and an arrangement with a combination barrier type. The potential barriers used include GaSb, GaAs, and AlAs. So that with the triple potential barrier model, there are 9 arrangements, namely 3 uniform arrangements and 6 combination arrangements.

3.2.1. Uniform arrangements. In a uniform arrangement, the following transmission coefficient values are obtained. In this case, A is a GaSb semiconductor, B is a GaAs semiconductor, and C is an AlAs semiconductor. From Table 4.1, the greater energy of the electron does not make the transmission coefficient bigger. In the uniform GaSb barrier potential arrangement, the transmission coefficient value can reach a maximum value of 1,000, meaning that at 0.49 eV electron energy, all electrons can pass through the potential barrier. This is because GaSb has a potential energy value of $V < E_{maks}$. In addition, a uniform arrangement of potential barriers causes resonance so that the probability of electrons passing is greater until it reaches a maximum. Furthermore, in the formation of the GaAs uniform barrier potential, the maximum coefficient value is 0.9797. In the AlAs arrangement, the transmission coefficient value only reaches 0.2809. From these results it can be seen that when the potential energy value of the barrier is greater, the value of the transmission coefficient is getting smaller.

Table 4.1 Transmission coefficients in the uniform arrangement

Electron Energy (eV)	T		
	AAA	BBB	CCC
0.005	0.005	0.000	0.000
0.490	1.000	0.1561	0.0009
0.585	0.9484	0.4981	0.0021
0.744	0.896	0.9797	0.0095
1.000	0.9688	0.7564	0.2809

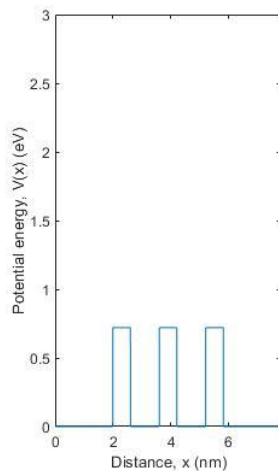


Figure 2. Triple potential barrier of GaSb.

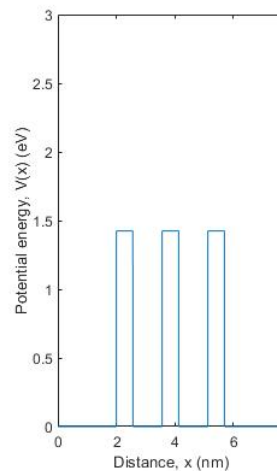


Figure 3. Triple potential barrier of GaAs.

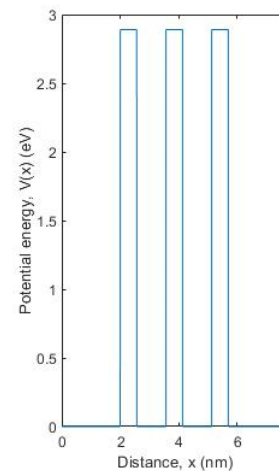


Figure 4. Triple potential barrier of AlAs.

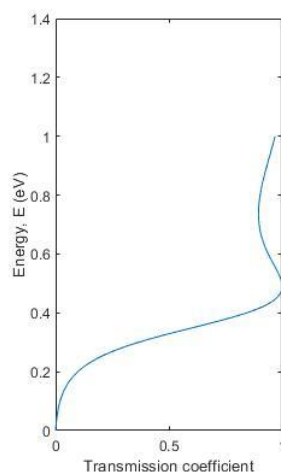


Figure 5. The transmission coefficient on the triple potential barrier of GaSb.

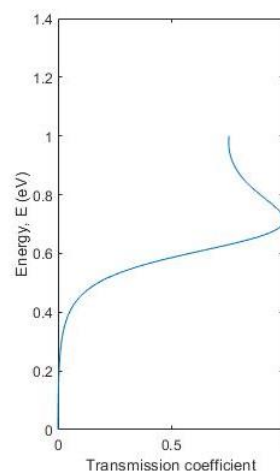


Figure 6. The transmission coefficient on the triple potential barrier of GaAs

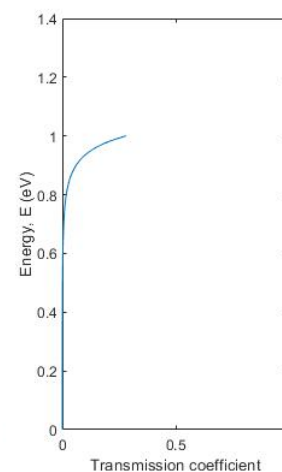


Figure 7. The transmission coefficient on the triple potential barrier of AlAs

Figure 5 until figure 7 shows the results of the simulation on the triple potential barrier A, B, and C. It can be seen that the transmission coefficient increases with increasing electron energy until it reaches a maximum value before decreasing the coefficient. If you look further, the transmission coefficient on GaSb can reach a maximum value of 1,000, while the GaAs and AlAs are not up to 1. The transmission coefficient reaches a maximum value after experiencing a significant increase, but then decreases. This decrease occurs because the basic function of the transmission coefficient is in the form of hyperbolic trigonometry which causes the transmission coefficient to be periodic. At some point, the value will reach a maximum then drop to a minimum and will rise again. In the combination arrangement there is one of the barrier potentials whose magnitude $E > V$, this results in resonance. This resonance phenomenon causes the transmission coefficient to be close to 1 or even 1 at certain electron energies because it is caused by one potential barrier affecting the other potential barrier and this also occurs because the three potential walls are symmetrical.

3.2.2. Combination arrangements. At the triple potential barrier with a combination arrangement, the value of the transmission coefficient varies even though the barrier is composed of the same 3 types of material. In this case, A is a GaSb semiconductor, B is a GaAs semiconductor, and C is an AlAs semiconductor.

Table 4.2 Transmission coefficients in combination arrays.

Electron Energy (eV)	T					
	ABC	CBA	CAB	BAC	BCA	ACB
0.005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.490	0.0641	0.0641	0.2004	0.2004	0.0398	0.0398
0.585	0.1594	0.1594	0.5996	0.5996	0.0896	0.0896
0.744	0.3541	0.3541	0.2659	0.2659	0.2972	0.2972
1.000	0.4425	0.4425	0.2239	0.2239	0.7939	0.7939

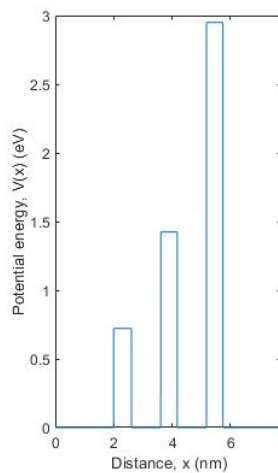


Figure 8. Triple potential barrier of ABC.

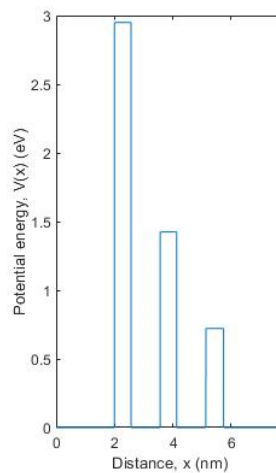


Figure 9. Triple potential barrier of CBA.

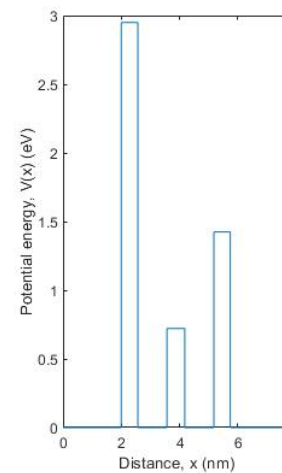


Figure 10. Triple potential barrier of CAB.

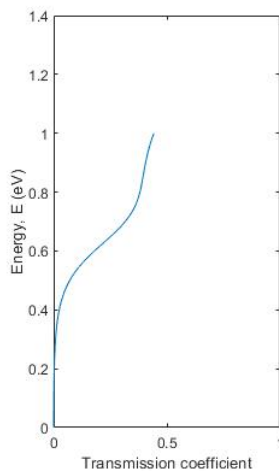


Figure 11. The transmission coefficient on the triple potential barrier of ABC.

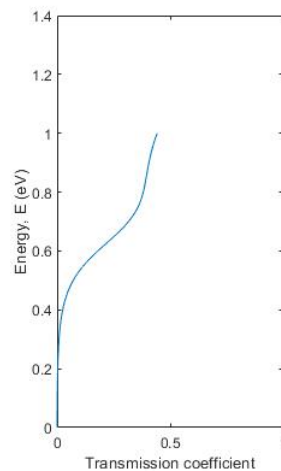


Figure 12. The transmission coefficient on the triple potential barrier of CBA.

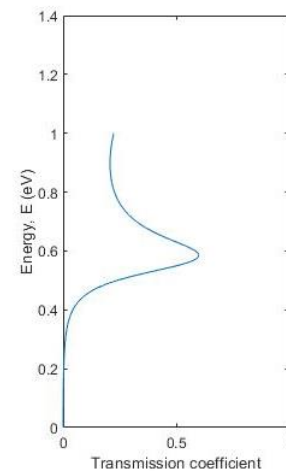


Figure 13. The transmission coefficient on the triple potential barrier of CAB.

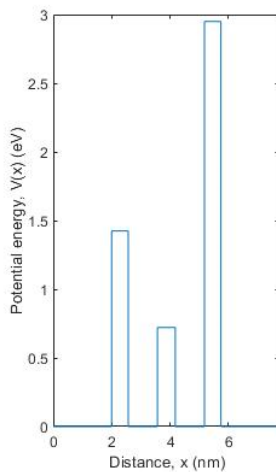


Figure 14. Triple potential barrier of BAC.

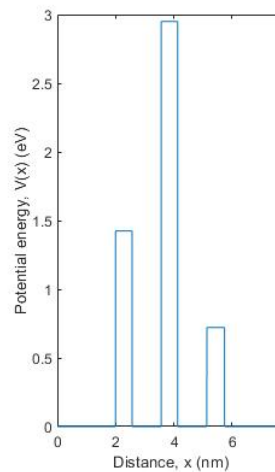


Figure 15. Triple potential barrier of BCA.

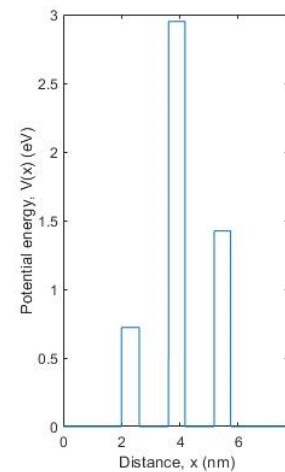


Figure 16. Triple potential barrier of ACB.

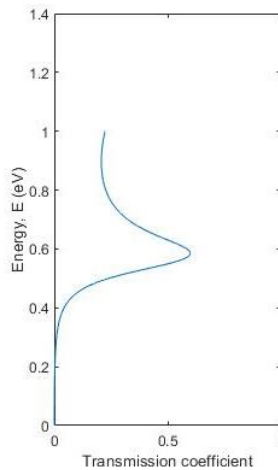


Figure 17. The transmission coefficient on the triple potential barrier of BAC.

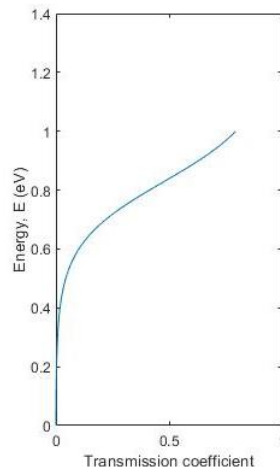


Figure 18. The transmission coefficient on the triple potential barrier of BCA.

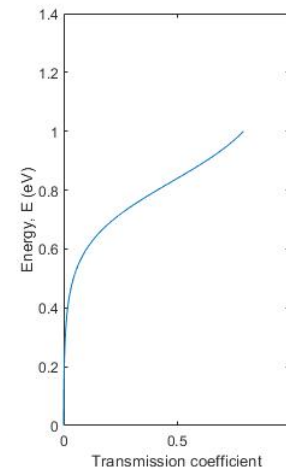


Figure 19. The transmission coefficient on the triple potential barrier of ACB.

Based on the figure and table above, it can be seen the value of the transmission coefficient on the combinatorial arrangement. It can be seen that there are 3 kinds of transmission coefficient values from 6 combination arrangements. Where 2 reverse combination arrangements show the same transmission coefficient value. That is, the transmission coefficient value of ABC is identical to CBA, CAB is identical to BAC, and BCA is identical to ACB. The largest transmission coefficient value is 0.7939 at the BCA and ACB arrays, this value corresponds to the electron energy of 1 eV. Furthermore, in the CAB and BAC arrangements, the largest transmission coefficient value is 0.5995 when the electron energy is 0.585 eV. And the value of the transmission coefficient in the ABC and CBA arrangements is 0.4425 when the electron energy is 1 eV. So that the arrangements that are more effective for generating large transmission coefficient values are BCA and ACB. Even though the 6 combinations consist of the same 3 semiconductor materials, it turns out that different arrangements produce different transmission coefficient values.

4. Conclusion

It can be concluded that the potential barrier arrangement affects the transmission coefficient value. In the uniform barrier arrangements, the value of the transmission coefficient decreases with increasing

potential barrier energy. The maximum transmission coefficient value in the uniform arrangement is 1.000 in the triple potential barrier of GaSb at 0.49 eV electron energy. In this state all electrons can pass through the potential barrier. Whereas in the arrangement of different barrier combinations, two opposing combination arrangements have the same transmission coefficient value. Thus from 6 combination arrangements, there are 3 kinds of transmission coefficient values. The largest transmission coefficient value is 0.7939 at the BCA and ACB arrays, this value corresponds to the electron energy of 1 eV.

Acknowledgments

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