Transmission Coefficient of Triple Potential Barrier Combination Structure Using Two-Dimensional Schrodinger Equation

Bambang Supriadi(✉), Tamara Pingki, Hana Mardhiana, Nurul Faridah, Elma Tri Istighfarini, and Subiki

Physics Education Department, University of Jember, Jember, Indonesia
{bambangsupriadi.fkip,subiki.fkip}@unej.ac.id

Abstract. Electronic devices that are made from semiconductors have made a lot of progress in the size of basic components that are more practical and effective, meaning that the size is getting smaller with greater data storage. The progress of these electronic devices cannot be separated from the tunneling effect phenomenon. In the study of quantum physics, a particle with a smaller energy E has a probability of breaking through the potential barrier V. The magnitude of the probability to break through is called transmission coefficient. The purpose of this study was to find the largest transmission coefficient value from the combination of semiconductor materials using the two-dimensional Schrodinger equation. The materials used are III-V alloy semiconductors, that is AlSb, GaP and InAs. Semiconductor materials will be arranged to form a triple potential barrier and will be analyzed numerically using Matlab R2022a. In this study, the maximum energy of an electron is 1 eV. The results showed that the potential barrier structure has an effect on the value of the transmission coefficient. In different combinations of barriers, the two opposite combinations have the same transmission coefficient. The maximum transmission coefficient value is 1000 at the triple potential barrier with ABC and CBA arrangement of 0.3038 eV.

Keywords: Transmission Coefficient · Schrodinger Equation · Semiconductor

1 Introduction

The period of classical physics occurred in the range of 1600 to 1890s which was dominated by Newtonian classical mechanics and Maxwellian electromagnetic wave theory managed to explain almost all the experimental results of science at that time [10]. In solving classical physics, there are differences in treatment between particles and waves and there are limitations in the amount of energy. At the end of the 19th century, several microscopic phenomena were discovered that could not be explained through classical physics, namely the black body radiation spectrum, the photoelectric effect, and the Compton effect [8]. Maxwell's theory of electromagnetic waves, which explained that light is malarly distributed in the form of electromagnetic waves, has hit a dead end so that the classical physics paradigm is experiencing a crisis [18].

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Microscopic phenomena that cannot be explained using classical physics theory gave birth to modern physics concepts. Modern physics studies the behavior of particles and waves on the atomic scale and subatomic particles or waves that move at high speeds. In 1900, Max Planck explained that energy can be divided into several packages or quanta which can explain the distribution of the intensity of radiation emitted by black bodies [6]. In 1905, Albert Einstein explained that light energy comes in the photoelectric effect in the form of quanta called photons [2]. Then in 1924, Arthur H. Compton observed changes in the wavelength of X-rays after being scattered by free electrons and the results showed that X-rays, which are considered as waves, also have particle properties [15]. After successfully explaining the photoelectric effect and the Compton effect, there is a de Broglie hypothesis which assumes that wave-particle dualism does not only belong to light, but also to particles. The de Broglie wavelength of a particle can be formulated as follows.

$$\lambda = \frac{h}{p} = \frac{h}{mv} \tag{1}$$

where m is the mass of the particle moving with speed v.

Erwin Schrodinger in 1887–1961 explained that when electrons move, waves are created which are de Broglie standing waves which produce solutions in the form of trigonometric or exponential functions [13]. The solution is a function or wave equation which is now known as the Schrodinger equation. The Schrodinger equation is a second-order differential equation that fulfills 3 conditions, namely obeying the law of the conservation of energy, not violating de Broglie's hypothesis, and good behavior (finite, single, and continuous) [4].

Semiconductor-based electronic devices have made a lot of progress in terms of basic component sizes that are increasingly practical and effective, meaning that component sizes are getting smaller with larger data stores. Initially, electronic devices such as televisions, computers, and laptops used vacuum tubes as their basic components. Over time, the use of diodes and transistors in *Integrated Circuits (IC)* affects the size of the basic components of electronic devices which are getting smaller to the nanometer scale with increasingly extraordinary performance [3]. The progress of these electronic devices cannot be separated from the phenomenon of the tunneling effect. According to the theory of classical mechanics, if a particle with energy E propagates and encounters a potential V whose value is greater, then the energy will be reflected back in the opposite direction [14]. But in the theory of quantum mechanics this is not the case, precisely when an energy E meets a potential V whose value is greater, then that energy has the probability to penetrate the potential [2]. This ability can occur because the wave nature will dominate over the particle nature. The probability of breaking through a potential barrier is called the transmission coefficient [12].

Determination of the value of the transmission coefficient can be analyzed through several methods, namely the Schrodinger equation, matrix propagation, and WKB (Wentzel-Kramers-Brillouin). The matrix propagation method has been widely used in several studies, one of which is research on the transmission coefficient on triple potential barriers of GaN, SiC and GaAs materials which produced the largest transmission coefficient of 0.819 [17]. In addition, there is also research which produces the largest transmission coefficient of 1.00 at an energy of 0.9200 eV [11] and research with a quadruple barrier potential on graphene material produces the largest transmission coefficient is 1.00 when the electron energy is 0.7500 eV [7]. Another research showing that the largest transmission coefficient value is 0.7939 in the BCA and ACB arrangement with an electron energy of 1.000 eV [16] and the largest transmission coefficient value is 0.8087 in the ADCB and BCDA arrangements, where A is GaSb, B is GaAs, and C is AlAs [9].

Not too many studies have used the Schrodinger equation to find the value of the transmission coefficient of a certain composition of materials. Therefore, this research will be conducted using the separation of variables in the two-dimensional Schrodinger equation. The reason for using the two-dimensional Schrodinger equation is because waves have the property of refraction, so that particles (electrons) also have the property of refraction. This result in the bias angle being one of the factors that greatly influences the motion of electrons which also affects electrons carrying out a transmission. In addition, the Schrodinger equation also does not ignore the physical meaning so that it can be easily applied, in contrast to the purely mathematical matrix propagation method [1].

Specifically, the materials used in this study are III-V alloy semiconductors, namely Aluminum antimonide (AlSb), Gallium phosphide (GaP) and Indium arsenide (InAs). AlSb has indirect and direct band gaps of 1.6 eV and 2.22 eV and has a lattice constant of 0.61 nm [19]. AlSb is a semiconductor material suitable for application in transistors and PN junction diodes because it has a large band gap [20]. GaP has an indirect band gap of 2.26 eV with a barrier width of 0.545 nm and is an important photonic material commonly used as an active ingredient in green light-emitting diodes [5]. While materials InAs has a bandgap of 0.354 eV and has a barrier width of 0.606 nm. InAs is used as a promising material for gas sensors, high-speed transistors, infrared photodetectors, and the manufacture of diode lasers [21]. The selected semiconductor materials will be arranged according to the predetermined combinations so as to form a potential triple barrier structure. This combination arrangement will be analyzed to obtain the largest transmission coefficient value using the Matlab R2022a computer program.

2 Transmission Coefficient

Semiconductor materials, namely AlSb, GaP and InAs have different energy gaps and wide potential barriers. The transmission coefficient possessed by electrons to penetrate the barrier in the tunneling effect can be analyzed using the two-dimensional Schrodinger equation. This method is carried out by using the separation of variables in the two-dimensional Schrodinger equation. Figure 1 shows a two-dimensional barrier model, but for incoming waves it only comes from one axis, namely the x-axis.

From the picture above, the general wave equation in area 1 to area 7 is

$$\Psi_1(x, y) = Ae^{ik_1(x+y)} + Be^{-ik_1(x+y)} \tag{2}$$

$$\Psi_2(x, y) = Ce^{ik_2(x+y)} + De^{-ik_2(x+y)} \tag{3}$$

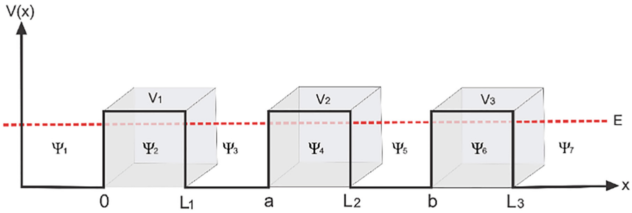

Fig. 1. Triple potential barrier in two-dimension.

$$\Psi_3(x,y) = Fe^{ik_1(x+y)} + Ge^{-ik_1(x+y)} \tag{4}$$

$$\Psi_4(x,y) = He^{ik_3(x+y)} + Ie^{-ik_3(x+y)} \tag{5}$$

$$\Psi_5(x,y) = Je^{ik_1(x+y)} + Me^{-ik_1(x+y)} \tag{6}$$

$$\Psi_6(x,y) = Ne^{ik_4(x+y)} + Oe^{-ik_4(x+y)} \tag{7}$$

$$\Psi_7(x,y) = Pe^{ik_1(x+y)} \tag{8}$$

with

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \tag{9}$$

and

$$k_2 = k_3 = k_4 = \frac{\sqrt{2m(V-E)}}{\hbar} \tag{10}$$

The above equation is the main reference for continuing calculations using the existing provisions on the nature of wave propagation, where waves propagate and penetrate a two-dimensional barrier. Based on the calculations performed using the two-dimensional Schrodinger equation, the t equation can be obtained as follows:

$$t_1 = \frac{4ik_1k_2e^{-2ik_1a}}{(k_2+ik_1)(ik_1+k_2)e^{-2k_2a} + (k_2-ik_1)(ik_1-k_2)e^{2k_2a}} \tag{11}$$

$$t_2 = \frac{4ik_1k_3e^{-2ik_1b}}{(k_3+ik_1)(ik_1+k_3)e^{-2k_3a} + (k_3-ik_1)(ik_1-k_3)e^{2k_3b}} \tag{12}$$

$$t_3 = \frac{4ik_1k_4e^{-2ik_1c}}{(k_4+ik_1)(ik_1+k_4)e^{-2k_4c} + (k_4-ik_1)(ik_1-k_4)e^{2k_4c}} \tag{13}$$

and the r equation as follows

$$r_1 = \frac{(k_2+ik_1)(ik_1-k_2)e^{-2k_2a} + (k_2-ik_1)(ik_1+k_2)e^{2k_2a}}{(k_2+ik_1)(ik_1+k_2)e^{-2k_2a} + (k_2-ik_1)(ik_1-k_2)e^{2k_2a}} \tag{14}$$

$$r_2 = \frac{(k_3 + ik_1)(ik_1 - k_3)e^{-2k_3a} + (k_3 - ik_1)(ik_1 + k_3)e^{2k_3b}}{(k_3 + ik_1)(ik_1 + k_3)e^{-2k_3a} + (k_3 - ik_1)(ik_1 - k_3)e^{2k_3b}} \tag{15}$$

$$r_3 = \frac{(k_4 + ik_1)(ik_1 - k_4)e^{-2k_4c} + (k_4 - ik_1)(ik_1 + k_4)e^{2k_4c}}{(k_4 + ik_1)(ik_1 + k_4)e^{-2k_4c} + (k_4 - ik_1)(ik_1 - k_4)e^{2k_4c}} \tag{16}$$

as well as the *p-value* as follows

$$p = \frac{\left((k_3 - ik_1)(ik_1 - k_3)e^{-2k_3b} + (k_3 + ik_1)(ik_1 + k_3)e^{2k_3b}\right)}{4ik_1k_3e^{-2ik_1b}} \tag{17}$$

All known equations are calculated manually using long substitution and elimination methods taking into account the wave function passing through the barrier. So that we can obtain the transmission equation for the three barriers, that is

$$T = \left| \frac{t_1t_2t_3}{\left(1 - r_3e^{2ik_1L_2}r_2\right) - \left(r_2 + r_3t_2e^{2ik_1L_2}p\right)e^{2ik_1L_1}r_1} \right|^2 \tag{18}$$

3 Result and Discussion

In the triple potential barrier with the combined arrangement, the value of the transmission coefficient varies even though the barrier consists of the same 3 types of material. In this case, A is an AlSb semiconductor, B is a GaP semiconductor, and C is an InAs semiconductor. In this study there were only six combination arrangements because the materials used amounted to 3 (3! = 6). The combinations are ABC, CBA, BAC, CAB, ACB, and BCA. After being analyzed numerically using Matlab R2022a, the results obtained are written in Table 1.

From the table, the graph of each combination arrangement is shown as follows (Figs. 2, 3, 4, 5, 6, and 7).

Table 1. Tranmission coefficient for triple potential barrier with schrodinger equation

E (eV)	*T* in Combinations Array					
	ABC	CBA	BAC	CAB	ACB	BCA
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.450	0.0012	0.0012	0.0014	0.0014	**0.3838**	**0.3838**
0.475	0.0016	0.0016	0.0019	0.0019	0.1282	0.1282
0.925	0.1222	0.1222	0.0969	0.969	0.0260	0.0260
0.950	0.1621	0.1621	0.1266	0.1266	0.0342	0.0342
0.975	0.2196	0.2196	0.1696	0.1696	0.0467	0.0467
1.000	**0.3038**	**0.3038**	**0.2333**	**0.2333**	0.0667	0.0667

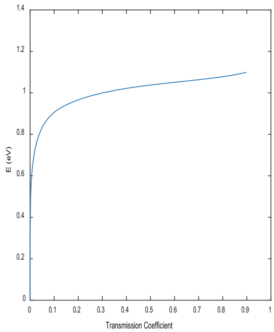

Fig. 2. Transmission coefficient of ABC arrangement.

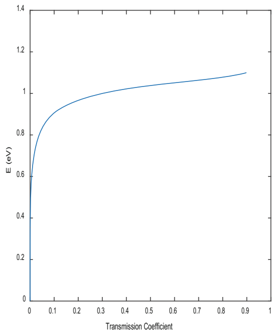

Fig. 3. Transmission coefficient of CBA arrangement.

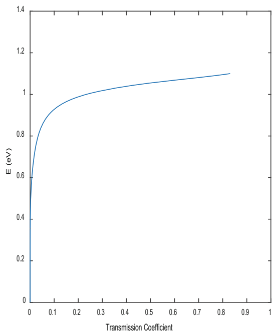

Fig. 4. Transmission coefficient of BAC arrangement.

In this study, the formula that used is very long because it uses the Schrodinger equation manually, both for analytical and numerical calculations. The maximum energy of electrons is 1 eV. The results show that reverse order has the same value, ABC and BAC arrangements have the same function graphs, CAB and CBA arrangements have the same function graphs, ACB and BCA arrangements have the same function graphs. So it

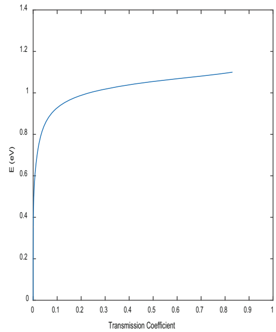

Fig. 5. Transmission coefficient of CAB arrangement.

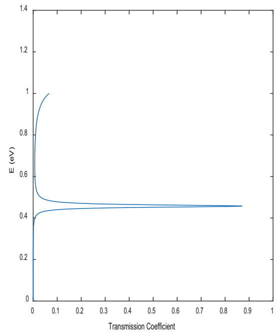

Fig. 6. Transmission coefficient of ACB arrangement.

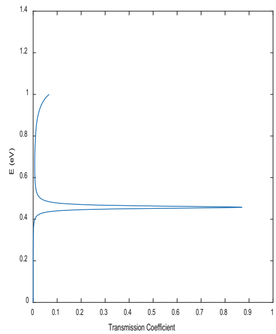

Fig. 7. Transmission coefficient of BCA arrangement.

can be seen that there are 3 kinds of transmission coefficient values from 6 combination arrangements. The number of combinations is in accordance with research [16], it's just that the materials used are different, so the shape of the graph and the coefficient values are also different, but both have 3 kinds of transmission coefficient values.

When the energy E continues to increase, the transmission coefficient increases slowly and when the energy E is at 0.900 eV and above, there is a considerable increase until E is 1.000 eV. When the E value is 1.000, the ABC and CBA arrangements have the same transmission coefficient value, which is 0.3038. While the BAC and CAB arrangement has the largest transmission coefficient value, that is 0.2333. The ACB and BCA arrangement the highest transmission coefficient value is obtained when the E value is 0.450 which is equal to 0.3838.

The ACB and BCA layouts have a different chart shape, where the charts have very large increases at almost half of the E value and then decrease very large and start to rise again until the E value is 1.000. This is because the composition of the material has a very large difference in potential energy from each barrier. ACB itself has a potential energy arrangement of 1.6, 0.354, 2.26. While the potential energy composition of the BCA composition is 2.26, 0.354, 1.6. This is clearly a new thing because in previous research, however the arrangement of the barriers, it must have produced a function graph that has almost the same shape. These results indicate that if there is a significant decrease in the barrier potential value from the first barrier to the second barrier and a significant increase in the barrier potential value from the second barrier to the third barrier, or vice versa, this can have a large impact on the resulting graph function.

In general, the factors causing the differences in the graphs are the differences and the placement of the composition of the materials, which do go up and down significantly. This is supported by other graphs which have almost the same shape because the potential barrier which is very small is located in front or behind which does not really affect the flow of energy from the first barrier potential to the second barrier potential and from the second barrier to the third barrier potential. These results are also almost the same as research [16] on the CAB and BAC arrangements (A is GaSb, B is GaAs, and C is AlAs), where there are two conditions, namely an increase and decrease in the value of the transmission coefficient even when it has not reached 1 eV energy, but this happens quite slowly, and the energy difference E is quite large. In contrast to research [16], the results of the research conducted this time can be seen that the increase and decrease occurs very quickly with a relatively small energy difference.

4 Conclusion

It can be concluded that the arrangement of potential barriers affects the value of the transmission coefficient. In different barrier combination arrangements, the two opposing combination arrangements have the same transmission coefficient value. The largest transmission coefficient value is 0.3838 in the ACB and BCA arrangement at an electron energy of 0.450 eV. The barrier potential which has a very small value will affect the graph of the function if it is placed in the middle of the array.

Based on the results and conclusions that have been obtained, the authors suggest that further research can use other methods to analyze the transmission coefficient and use alloy semiconductor materials which have enormous potential in the development of electronic devices that are beneficial to the world. The use of other solving methods can be a significant development in quantum physics because the study is clearly different, from particle behavior, particle dimensions and barrier materials, how to calculate, to the final result. There are many methods to find the value of this transmission coefficient, either using the Propagation Matrix or WKB (Wentzel-Kramers-Brillouin) method for two dimensions and higher dimensions. Potential barriers can also be multiplied by four or more which can be analyzed in uniform barrier arrangements and in combinational arrangements.

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