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Tunneling effect on double potential barriers GaAs and PbS

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Tunneling effect on double potential barriers GaAs and PbS

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Abstract. A simple model of transport phenomenon tunnelling effect through double barrier structure was developed.In this research we concentrate on the variation of electron energy which entering double potential barriers to transmission coefficient. The barriers using semiconductor materials GaAs (Galium Arsenide) with band-gap energy 1.424 eV, distance of lattice 0.565 nm, and PbS (Lead Sulphide) with band gap energy 0.41 eV distance of lattice is 18 nm. The Analysisof tunnelling effect on double potentials GaAs and PbS using Schrodinger's equation, continuity, and matrix propagation to get transmission coefficient. The maximum energy of electron that we use is 1.0 eV, and observable from 0.0025 eV- 1.0 eV.The shows the highest transmission coefficient is0.9982 from electron energy 0.5123eV means electron can pass the barriers with probability 99.82%. Semiconductor from materials GaAs and PbS is one of selected material to design semiconductor device because of transmission coefficient directly proportional to bias the voltage of semiconductor device. Application of the theoretical analysis of resonant tunnelling effect on double barriers was used to design and develop new structure and combination of materials for semiconductor device (diode, transistor, and integrated circuit).

1. Introduction

A familiar fact of quantum Physics is about microscopic system on small size scale, the interaction between atoms and charge. This certainly holds on nanometres-size of a Bohr radius ~ 0.5 Å (0.05 nm).The concept of tunnelling effect is quantum mechanical phenomenon which focus on particle can pass through potentials barriers well even when classically don'thave the energy to do $\boldsymbol{E} < \boldsymbol{V_0}$. In Tunnelling effect we consider the wave nature of the electron to describe its interaction with series of potential Barriers [3]. In tunnelling double barriers occurs resonant condition. Resonant tunnelling of nonequilibrium double barriers as obtained by injection with a ballistic launcher [1]. The application of tunnelling effect is responsible for many important research areas such as development of semiconductor device, photovoltaic cell and imaging (scanning tunnelling microscopy). General application of tunnelling effect is the design of TFET (tunnel field-effect transistor) which has been recognized as feasible choice since its subshreshold swing at room temperature is able to be less than 60mV/decade which is a physical limit of conventional MOSFET(metal oxide semiconductor filed effect transistor) [2]. Quantum confined structures on the nanometer scale, such as quantum wells, wires or dots, have been increasingly used as active components in novel optical and electrical devices, including lasers, photodetectors, and photovoltaics [7]. Materials that exhibit quantum confinement tend to have remarkable thermal, optical and electronic properties useful in many nanotechnology-based applications [6]. In this research we combine two kinds semiconductor device and simulated to give information about tunnelling pheneomenon. Atomistic and quantum simulation are necessary to study carrier transport at nano scale [10].

With continuous scaling of semiconductor devices, it is valuable to study material electronic properties and device transport characteristics at the atomic level [9]. The theoretical analysis application of tunneling effect isto obtain information about process in order toprove the formulation and investigating tunneling effect of GaAs (Gallium Arsenide) and PbS (lead sulphide) on double potentials (resonant tunnelling). Analysis of tunneling effect start from defining equation for each condition before strike the barrier, in barrier, and after pass barrier[4]. Second, find the *k vector* by comparingthe electron energy and “height” of barrier. Third, get the wave equations for each condition using continuity of state. The last is arranging complete equation to solve the Transmission and Reflection of wave function. On Single Potential is easy to find another characteristic of Tunneling effect, we just finish three step above to find it.On the contrary, indouble potential barriers of asymmetric potential, this step is difficult because we have five wave function from double potentials in this condition. Another solution is easier to solve the problems in multiple potentials using matrix propagation to solve equation and get transmission coefficient. Transmission coefficient determine the probability of the particle going through the barriers. Transmission coefficient also contribute to resistance of semiconductor materials. Because all semiconductor device are free from the resistance mismatch problem [5].

In this case we consider the analysis of Tunneling effect on double barriers, which consist of GaAs (Galium Arsenide) and Lead Sulphide (PbS).Characteristics of GaAs consist two kinds of atoms inclung Galium and Arsenide with band gapenergy of 1.424 eVand distance of Lattice is 0.565 nm as width of barriers. Device engineers are interested in GaAs because it is an example of III-V compound semiconductor that used to make laser diodes and high-speed transistors [7].PbS (lead Sulphide) consist of two kind atoms Lead (Pb) and Sulphide (S). Lead from group IV-A and Sulphide from VI-A has small band gap ~ 0.41 eV [11]. Bohr Radius excitation 18nm, and small effective mass from GaAs and lead Sulphide is $0.075m_0$[12],A few studies have been performed on films thinner than 20 nm as combination from semiconductor device[6]**.** In this research the film thinner about~ 19.565 nm from total thickness of GaAs and PbS,itis an attractive material for quantum confined structures. Combination between GaAs and PbS make a new tunnelling effect analysis and characterization to predict the value of transmission coefficient. Method of matrix propagation is one of the best method to solve tunnelling effect on another types of barrier for example: single barrier, symmetric multiple barrier, asymmetric multiple barrier, periodical barrier, sinusoid barrier, or combination of barrier [8].Transmission coefficient of electrons occurs on resonant tunnelling heterostructure double barriers has attracted much attention in recent years due the negative differential conductance behaviour [1].

2. Methods

Analysis of tunneling effect on GaAs andPbS begin by giving a potential shape definition. There are kinds of potentials shapes: single, double, multiple, and series potentials [8]. GaAs and PbS has different band gap energy, the shape of potential is asymmetric.We can calculate the propagation of matrix to find $\hat{p}_{step}$ consist of transmission and reflection coefficient. Both of them represent energy for each electron in different positions [8]. On multiple standardpotentials we can obtain the potential notation by using x_n for first potential, x_{n+1}, for second potential and according to figure 1, distance of first potential and second potentials are denoted by $L_n = (x_{n+1} - x_n)$.

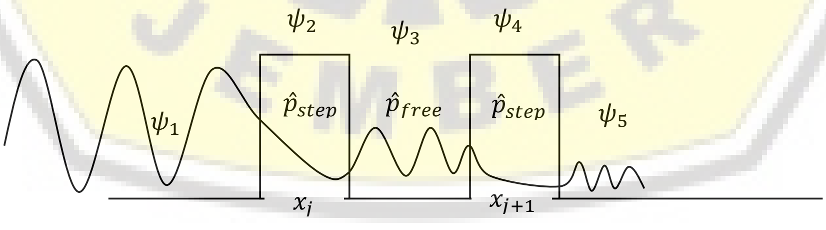

Figure 1. Tunneling in Double Potential Barriers [3]

Analysis and calculation propagation matrix n_{th} region can be solved by multiplying each region matrix $\hat{p}_{step}$ and $\hat{p}_{free}$become $\hat{p}_j = \hat{p}_{step} \cdot \hat{p}_{free}$. Two or more wave function must be continuous, this means that at potential step occur at the boundary between region$j$ and j_{th}. Energy of electron moving circular on atom can be describe as.

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

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Equation (1) is energy formulation with relation of k number [3],wave vector from particle (electron) before and after strike the potentials can be written as function of energy.

$$k = \frac{2m\,(E)^{1/2}}{\hbar} \; and \; k' = \frac{2m\,(E-V)^{\frac{1}{2}}}{\hbar} \quad (2)$$

The electron motion in microscopic condition can be described as wave function for each region on tunnelling effect can be define on equation (3) and (4) [11],ψ_j used forthe first potentials barriers' wave function and ψ_{j+1} for next barriers. There is no limit to use the barriers on analyse of tunnelling effect phenomena but in this research only use double barriers with different energy height.

$$\psi_j = A_j e^{ik_n x} + B_j e^{-ik_n x} \quad (3)$$

$$\psi_{j+1} = C_{j+1} e^{ik_{n+1} x} + D_{j+1} e^{-ik_{n+1} x} \quad (4)$$

Two wave function on each regionmust be continuous on tunnelling process.The analysis of continuity using first order derivation of wave function on equation (5).

$$\psi_n = \psi_{n+1}$$

$$e^{ik_n x} + B_n e^{-ik_n x} = C_{n+1} e^{ik_{n+1} x} + D_{n+1} e^{-ik_{n+1} x}$$

$$\frac{d\psi_n}{dx} = \frac{d\psi_{n+1}}{dx}$$

$$(ik_n)\, A_j e^{ik_n x} + (-\, ik_n) B_n e^{-ik_n x} = (ik_{n+1}) C_{n+1} e^{ik_{n+1} x} + (-\, ik_{n+1}) D_{n+1} e^{-ik_{n+1} x} \quad (5)$$

Equation (5) is the result of wave function derivation for each region and with simple process we can get equation (6) for grouping factor k_n and k_{n+1} (wave vector for each wave) [8].

$$(k_n A_j) e^{ik_n x} - k_n B_n e^{-ik_n x} = (k_{n+1}) C_{n+1} e^{ik_{n+1} x} + (-\, k_{n+1}) D_{n+1} e^{-ik_{n+1} x} \quad (6)$$

The Equation (7) divided by wave vectork_n, and we get eq (10) comparison between k_{n+1} *and* k_n.

$$A_n e^{ik_n x} - B_n e^{-ik_n x} = \left(\frac{k_{n+1}}{k_n}\right) C_{n+1} e^{ik_{n+1} x} - \left(\frac{k_{n+1}}{k_n}\right) D_{n+1} e^{-ik_{n+1} x} \quad (7)$$

Effective electron mass for simulation can describe as comparison between wave vector k_{n+1} and k_n

$$\left(\frac{k_{n+1}}{k_n}\right) = \left(\frac{m_n (k_{n+1})}{m_{n+1}\,(k_n)}\right)$$

The equation (6) and (7) can be combined and re-write into square-matrix approximation.

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} A_n \\ B_n \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \left(\frac{k_{n+1}}{k_n}\right) & \left(\frac{k_{n+1}}{k_n}\right) \end{bmatrix} \begin{bmatrix} (C_{n+1}) \\ (D_{n+1}) \end{bmatrix} \quad (8)$$

The Value of A_n *and* B_n from equation (8) can solve by using invers method of matrices to obtain matrices $\hat{p}_{step}$.

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = \underbrace{\frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ \left(\frac{k_{n+1}}{k_n}\right) & \left(\frac{k_{n+1}}{k_n}\right) \end{bmatrix}} \begin{bmatrix} (C_{n+1}) \\ (D_{n+1}) \end{bmatrix}$$

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = \hat{p}_{step} \begin{bmatrix} (C_{n+1}) \\ (D_{n+1}) \end{bmatrix}$$

$$\widehat{p}_{step} = \frac{1}{2}\begin{bmatrix}\left(1+\frac{k_{n+1}}{k_n}\right) & \left(1-\frac{k_{n+1}}{k_n}\right)\\ \left(1-\frac{k_{n+1}}{k_n}\right) & \left(1+\frac{k_{n+1}}{k_n}\right)\end{bmatrix} \quad (9)$$

Matrix propagation on potential step can express on equation (9). The same steps to findmatrices of$\hat{p}_{free}$can be obtained by using elimination factor of reflection wave from eq (10) and (11).

$$\psi\, A_n e^{ik_n x} = \psi_{cn} \quad (10)$$

$$\psi\, B_n e^{-ik_n x} = \psi_{Dn} \quad (11)$$

The result of matrix propagation operation identity appears and with invers matrix we can write on equation .

$$\begin{bmatrix} e^{ik_n x} & 0 \\ 0 & e^{-ik_n x}\end{bmatrix}\begin{bmatrix} A_n \\ B_n\end{bmatrix} = \begin{bmatrix}(C_{n+1})\\(D_{n+1})\end{bmatrix} \quad (12)$$

Simple expression of value A_n and $B_n$as amplitude from reflection wave express with equation (12)

$$\begin{bmatrix} A_n \\ B_n\end{bmatrix} = \begin{bmatrix} e^{-ik_n x} & 0 \\ 0 & e^{ik_n x}\end{bmatrix}\begin{bmatrix}(C_{n+1})\\(D_{n+1})\end{bmatrix}$$

$$\begin{bmatrix} A_n \\ B_n\end{bmatrix} = \hat{p}_{free}\begin{bmatrix}(C_{n+1})\\(D_{n+1})\end{bmatrix}(16)$$

$$\widehat{p}_{free} = \begin{bmatrix} e^{-ik_n x} & 0 \\ 0 & e^{ik_n x}\end{bmatrix} \quad (13)$$

Matrix propagation of $\hat{p}_{free}$from particle in outer of barriers can be written as equation (13). Scalar product for $\hat{p}_{free} \cdot \hat{p}_{step}$ can be written as $\hat{p}_{n-th\ region}$ as matrix propagation for amount of potential barriers.

$$\hat{p}_{free} \cdot \hat{p}_{step} = \hat{p}_{n-th\ region}$$

$$\widehat{p}_{n-th\ region} = \frac{1}{2}\begin{bmatrix}\left(1+\frac{k_{n+1}}{k_n}\right)e^{-ik_n x} & \left(1-\frac{k_{n+1}}{k_n}\right)e^{-ik_n x}\\ \left(1-\frac{k_{n+1}}{k_n}\right)e^{ik_n x} & \left(1+\frac{k_{n+1}}{k_n}\right)e^{ik_n x}\end{bmatrix} = \begin{bmatrix} P_{11} & P_{12} \\ P_{12}^* & P_{11}^*\end{bmatrix} \quad (14)$$

For multiple potential in general we can find$q$ potential step. Propagation matrix can be written as:

$$\hat{P} = \prod_{n=1}^{n=q} \hat{P}_n$$

Transmission of probability can be calculated by Determinant of matrix $\widehat{p}_{n-th\ region}$

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

$$T = \left(1 + \frac{1}{4}\frac{V_0}{E(E-V_0)} sin^2(k'L)\right) \quad (15)$$

The expression of transmission coefficient in other style can be written as function energy of particle E and potential barrier energy V_0 express on equation (19).

3. Result and Discussion

The simulation of tunneling effect on double potentials barriers GaAs and PbS shows by computer program. The aim of this research is analyzingthe value of transmission coefficient and the relation of semiconductor materials application.The value of transmission coefficient indicated probability of electron to pass the barriers higher, transmission coefficient making semiconductor materials easier to increase bias voltageon electronical device, because more electron on conduction band can moving easily. Simulation on computer programming of tunneling effect using maximum electron energy 1 eV and observable on computer simulation from 0.0025 eV - 1.0 eV because energy 0.0025 eV is the minimum value that can recorded on computer programming according to width of first potentials and second potentials. Effective electron mass is 0.075 m_0 from reduction electron mass. Energy for first and second barriers using bandgap energy 1.424 eV for GaAs, and 0.41 eV for PbS, the space between barriers using double Bohr radius (1.0 nm) to approach the general size of semiconductor layer~ 20 nm [6].

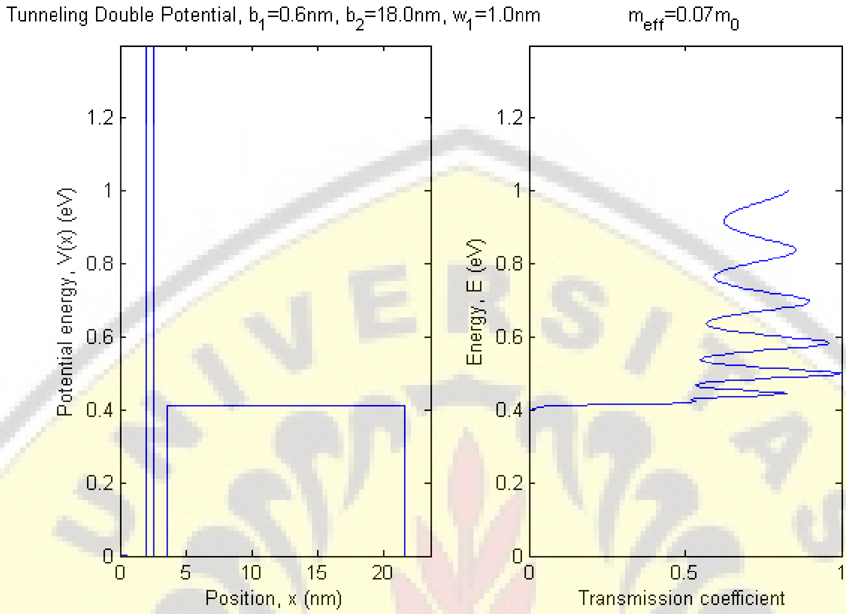

Figure 2. Result from ComputerSimulation (left side is model of double barriers and right side is relation between electron energy to transmission coefficient)

The result of simulation shows on figure 2withtwo pictures, left side isfirst potential of GaAs with band gap energy 1.424 eV barrier width 0.565 nm and the second barriers PbS band gap energy 0.41 eV and barrier width 18 nm.Figure 2 also explain about the relation between electron energy and transmission coefficient, according to equation (15) there are relations between electron energy to transmission coefficient, energy of electron on *(y-axis)* and transmission coefficient on *(x-axis)*. Analysis from figure 2 left side and right side explain the value of transmission coefficient make sinusoid graphic to electron energy, if electron strike double barriers with energy $E < V_0$, electron will pass the barriers even the classical mechanics don't do this, but in this condition electron that moving on microscopic scale has duality character asparticle and wave. In this case electron moving as wave, so if electron pass the barriers electron can penetrate barriers although electron energy less than barriers energy. Numerical result of tunnelling effect shows on table 1 and nine sample data were chosen from picture 2 on relative maximum transmission coefficient to approach maximum transmission coefficient.

Table 1. Energy of electron and Transmission coefisient

Data	Electron Energy (eV)	Transmission Coefficient
1	0.0025	$3.45 \cdot 10^{-17}$
2	0.3975	0.0035
3	0.4259	0.5229
4	0.4453	0.8249
5	0.5123	0.9982
6	0.5886	0.9616
7	0.6975	0.8993
8	0.8425	0.8524
9	1.0	0.8291

Data simulation from Table 1 as first peak graphic given electron energy 0.0025 eV with transmission coefficient is $3.45 \cdot 10^{-17}$, in this condition electron energy less than energy of barriers. Small energy electron on data number 1 try to penetrate double barriers because electron characteristic as wave can pass barriers in small transmission coefficient, because strike double potential with high potentials first and second potential is wide. Wide potential also give contribution on transmission coefficient, the wider of barriers will make small transmission coefficient [8].Second peak observable from data number 2 on table 1 with energy of electron is 0.3975 eV and transmission coefficient is 0.0035 means only 0.35% total of electron can pass the barriers, this data shows increasing of electron energy and transmission coefficient from data before. On simulation data number 1 until number 4, electron pass double barriers in resonant condition tunneling with double penetrate barriers. Data number 4 with electron energy 0.4453 eV and transmission of coefficient indicates that 0.8249 or 82.49% amount of electron can pass the barriers. Electron which pass the barriers on the limit of second barriers height 0.41 eV givenvalue transmission coefficient increase significantly from 0.5229 (data number 3) to 0.8249 (data number 4), this condition depend on type of potentials barriers shape, if energy of electron approach on the limitof double barrier on system barriers, electron more difficult to pass the barriers on wide potential size, because the probability of electron wave function decrease rapidly on second potentialsaccording to first potential.Datanumber 5 is the maximum value of transmission coefficient, proportion electron energy directly l to transmission coefficient, but on data number 5 and data number 6 although electron energy increase transmission coefficient is not directly proportional because wave factor*(k and k')* making important contribution to the transmission coefficient value.

Simulation from data number 6 until number 9, electron energy increase rapidly but transmission coefficient decrease. This condition happen because theoretical background of quantum mechanics, electron energy is bigger than second barriers but smaller than first barrier.This condition makes electrononly pass one barriers, but the second barrier also contributing to perturbation energy that influence of transmission coefficient. Maximum electron energy 1 eV on last data make the transmission coefficient value 0.8291 or 82.91% probability of electron can pass the barrier. The relation between energy and transmission coefficient also shows on figure 3 that explain nine dots on blue thick colour express nine transmission coefficient. Generally, transmission coefficient directly proportional withelectron energy from the curve on picture 3, but on special condition,transmission coefficient also depends on another variable of potential barriers (energy barrier, width of barrier, and distance between barriers).

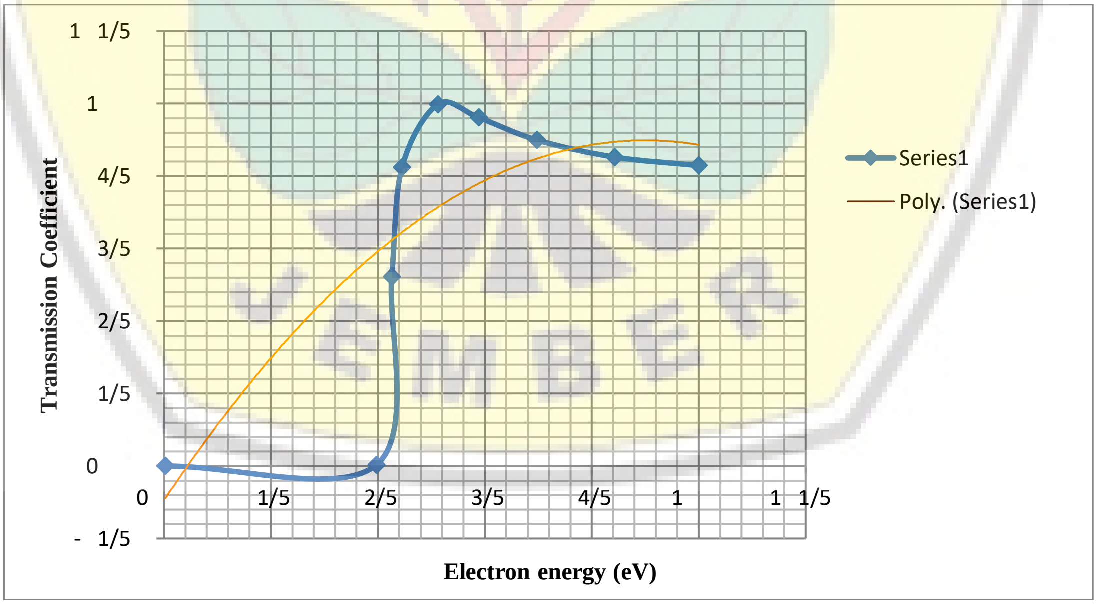

Figure 3. Relation energy with Transmission Coefficient

4. Conclusion

From the analysis result and tunnelling effect simulationon double barriers GaAs and PbS, themaximumnumber of transmission coefficient is 0.9982 or 99.82% on energy of electron0.5123 eVwhich indicates ideal condition, because maximum transmission coefficient reaches relative small energy related to small power consumption for electrical component based on semiconductor device.This research give information about combination of semiconductor materials (GaAs and PbS) in application tosemiconductor layerto design and develop diode, transistor and another semiconductor device like IC (integrated circuit) and computer processor. Analysis of tunnelling effect GaAs (gallium arsenide) and PbS (lead sulphide) ascombination of materials on semiconductor with transmission coefficient 99.82 % and small power consumption to move electron in order to pass the barriers and make electricity is suggested material for semiconductor device and also can give new information about theoretical analysis on Quantum Mechanics especially in tunnelling effect. On further research about tunnelling effect, we can expand analysis of tunnelling effect not only for double barriers but also on series barriers or shape of barriers on parabolic potentials.

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