DC ANALYSIS OF GAAS/ALAS SINGLE BARRIER ASYMMETRIC SPACER TUNNEL DIODE

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Abstract

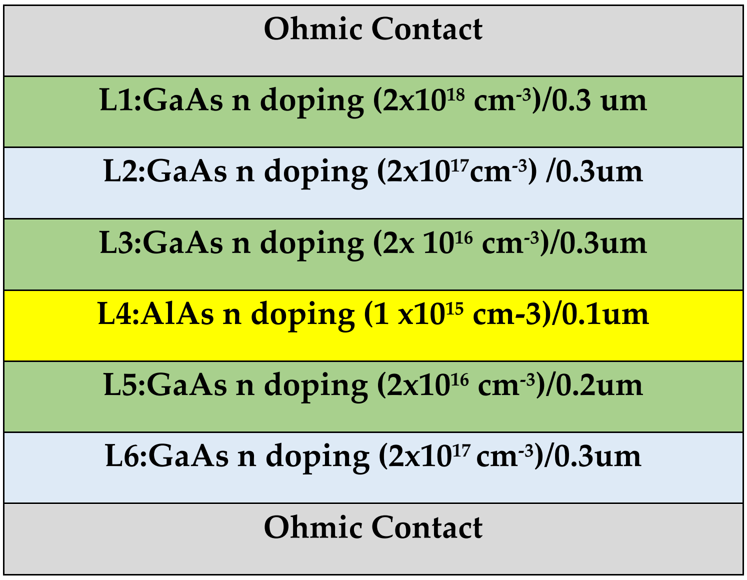
After Leo Esaki had reported the first tunnel diode in the early of 1960, there are development of Asymmetric Spacer Tunnel (ASPAT) diode. This device appears to have unique I-V characteristic, where it has zero turn on bias with minimum leakage current. Hence, with respect~~s~~ to this unique characteristics, this study will perform the physical modelling of Gallium Arsenide/ Aluminium Arsenide (GaAs/AlAs) of single barrier asymmetric spacer tunnel diode in COMSOL by considering all the parameters involved in designing the device such as the dimensions of ASPAT, the concentration, materials and numerical modelling involved. These parameters are significant in the calculation of current density when the device being applied with external voltage. At the end of this study, the I-V characteristics of ASPAT in COMSOL will be analysed and compared with the reported I-V characteristics of ASPAT diode in SILVACO to determine either it is reciprocated in terms of zero voltage switching and minimum reverse bias.

Keywords: *GaAs; AlAs; single barrier; asymmetric spacer tunnel diode.*

INTRODUCTION

In research from (Ariffin, 2019) asymmetric spacer tunnel (ASPAT) diode is one of the semiconductors that consists of zero turn on bias feature with a minimum leakage current. Realizing the unique characteristics that being shown by this device, it will consume a small value of voltage to turn on added with a low cost of fabrication in terminating the leakage current .The physical modelling of single barrier GaAs/AlAs of asymmetric spacer tunnel diode had successfully done in SILVACO and a study regarding on the DC analysis of the device had been achieved. Therefore, in this paper, the physical modelling of asymmetric spacer tunnel diode was done in COMSOL Multiphysics using semiconductor module, to solve the current density across heterojunction and the whole structure in order to produce the I-V characteristics of the device that is zero turn on feature with the minimum leakage current. After that, this study will analyse the I-V characteristics of ASPAT in COMSOL with SILVACO in terms of parameters involved with the relation of numerical modelling and voltage biased.

METHODOLOGY



Ohmic Contact

L1:GaAs n doping (2x10^{18} cm^{-3})/0.3 um

L2:GaAs n doping (2x10^{17}cm^{-3}) /0.3um

L3:GaAs n doping (2x 10^{16} cm^{-3})/0.3um

L4:AlAs n doping (1 x10^{15} cm-3)/0.1um

L5:GaAs n doping (2x10^{16} cm^{-3})/0.2um

L6:GaAs n doping (2x10^{17} cm^{-3})/0.3um

Ohmic Contact

Figure 1: Epitaxial Layer of ASPAT with the types of doping, concentrations and dimensions.

Figure 1 shows the epitaxial layer of single barrier GaAs/AlAs asymmetric spacer tunnel diode. By several modification of concentration from (Yang et al., 1993), the physical modelling of the device is being filled with n doping where layer one consists of GaAs with 2 × 10^{18} cm^{-3} concentration, layer two consists of GaAs with 2 × 10^{17} cm^{-3} concentration, layer three consists of GaAs with 2 × 10^{16} cm^{-3} concentration, layer four consists of AlAs with 1 x 10^{15} cm^{-3} concentration, layer five consists of GaAs with 2 × 10^{16} cm^{-3} concentration and layer six consists of GaAs with 2 × 10^{17} cm^{-3} concentration . Lastly, there are the ohmic contact at the top and bottom of the structure. By default, the ohmic contacts are being specified in the COMSOL package.

Table 1: Material Parameters for GaAs/ AlAs

Material Parameters	**GaAs**	**AlAs**
Relative permittivity	12.4	10
Band Gap (eV)	1.424	2.83
Electron Affinity (V)	4.07	3.01
Effective density of states, Conduction band, Nc (1/m^3)	4.7x10^{17}	1.5x10^{19}
Effective density of states, Valence band Nv (1/m^3)		
Electron Mobility (m2/Vs)	8.5	0.2
Electron Lifetime, SRH (ns)	1	1

Apart from that, the dimension is being set to the ratio of 40:1, that is the barrier needs to have a very thin layer in order to make sure the current can tunnel across hetero junction. Here, based on (Ariffin, 2019) the dimension of the spacer 1, spacer 2 that sandwich the barrier maintained with the asymmetric dimension, that is spacer one need to have a bigger dimension compared to spacer 2 . This is to make sure there will be an accumulation region during the band bending. Besides, the most significant element in physical modelling of ASPAT is the material, along with their respective parameters. The parameters of the materials have been manually defined. There are two materials have been used in the semiconductor which is the GaAs and AlAs , at 300K.The GaAs is being specified at all domains except domain four ,as the domain four is the barrier that being filled with AlAs The parameter for each GaAs is being shown in Table 1 based on (Sze et al., 2021), and the AlAs is also being stated based *on (Properties of III-V Semiconductors*)

It is crucial to determine the material used along with its parameters as it will affect the band gap of the structure. Besides, the material parameters also will be used in numerical modelling to solve the current density across hetero junction throughout thermionic field emission and thermionic emission, and current formulation across the whole structure of device by implementing the drift diffusion current. Therefore, it is important to know the effect of the materials used towards the device and the I-V characteristics. For instance, material parameters like electron affinity, which is the energy variance of an electron between the vacuum level and the bottom of the conduction band edge will determine the band discontinuities at semiconductor hetero interface, that is the ΔE_C and ΔE_V, as being illustrated by (Ariffin, 2019) in Figure 2. From the diagram, the electron affinity in AlAs is less than GaAs, hence, this difference will build up the band discontinuities and tunnel at the AlAs.

Figure 2: Energy band diagram of ASPAT Heterostructure

Apart from that, the effect of the other material parameters such as the effective density of states for valence band (E_v), effective density of states for conduction band (E_c), relative permittivity, electron mobility ,electron lifetime and energy band gap can be described from the numerical modelling. For instance, at the hetero junction, there will be the transfer of the electron from one type of material to another type of material. Based on the thermionic field emission numerical solution that involve at the boundary, the current density of J_{n1} is the current density for GaAs and Jn_2 is the current density for AlAs (Figure 3). From the numerical modelling, the GaAs contains the effective density of states in the conduction band that is higher than AlAs, thus, numerically it will consist the higher electron density, and higher current density compared to AlAs. Therefore, the electron will move from GaAs to AlAs, but the direction is being determined by the voltage applied to the device. However, for electron mobility, it is being used in the drift diffusion formulation. Based on numerical modelling of drift diffusion, the electron mobility will be calculated for the drift diffusion model. As the electron mobility for GaAs is higher than AlAs, the electron will drift from GaAs to AlAs.

NUMERICAL MODELLING: TRANSMISSION PROBABILITY OF ELECTRON

In quantum mechanics, the transmission probability of the electron through the heterojunction can be described by using Wentzel - Kramer's - Brillouin method, or WKB approximation method. WKB approximation is a useful method in order to obtain the approximate form of the tunnelling probability or transmission coefficient of the electron. Based on (Yang et al., 1993) the transmission coefficient can be calculated as shown in the equation 1 below.

$$T(E_x) = \begin{cases} exp(-4\pi/h \int_0^{X_E} [2m_n^*\{E_c(x) - E_x\}]^{\frac{1}{2}} dx) \\ if\ E_{min} \leq E_x \leq E_c(0+) \\ if\ E_c\ (0+) \leq E_x \end{cases} \qquad \text{Equation} \quad (1)$$

From the Equation 1, *h* is the Planck constant, m^*_n is the electron effective mass, E_x is the energy component in the x direction, E_{min} = max [$E_c(0^-)$, $E_c(W)$] and E_c is the energy at the conduction band.

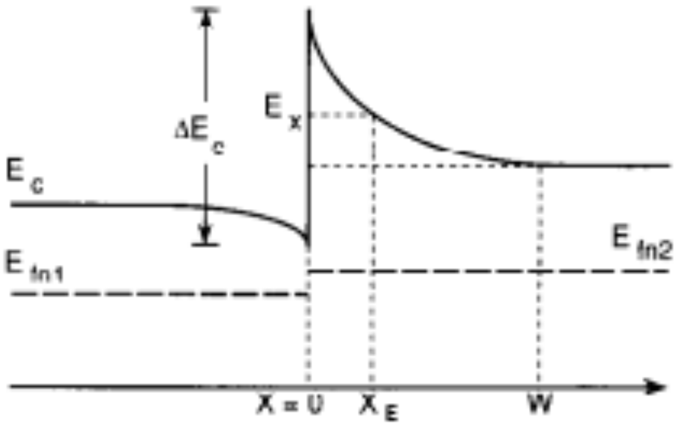


Figure 3: Schematic band diagram of an abrupt heterojunction. $Ef_{n1,2}$ is the electron quasi- Fermi level for semiconductor region 1 and 2

The illustration of the energy can be observed in the **Error! Reference source not found.** . From the illustration below, the tunnelling probability will be calculated across potential barrier from X = 0 to the X_E range. If the energy of electron in the range of E_{min} and $E_c(0^+)$, then the tunnelling probability will be from 0 to 1, but if the electrons energy is more that potential energy, $E_c(0^+)$, then, the electrons will across the barrier by thermionic emission instead of tunnel across it.

NUMERICAL MODELLING: THERMIONIC EMISSION AND THERMIONIC FIELD EMISSION ACROSS HETEROJUNCTION.

In the tunnelling phenomena, the carriers will tunnel across the hetero junction in the structure of the semiconductor and thus, this movement will lead to the measurement of I-V characteristics. The movements across the junction need to be considered in terms of their density. The electron and hole current density, J_n and J_p across the hetero junction will be calculated using the thermionic field emission boundary condition formulation, by considering the net exchange of the carriers. However, in this project, there is only n doping that will be used thus the solutions towards the net exchange of carriers in terms of holes is negligible. Based on (Yang et al., 1993), by using the Boltzmann energy distribution, the density of electron current J_n across the heterointerface is arising from the net exchange of electron between different materials, that is GaAs and AlAs as being stated in Equation 2 below.

$$J_{n1}(0^-) = -qV_{n1}(1+d)\, n_1(0^-) \exp\left(\frac{-\Delta Ec}{kT}\right) \qquad \text{Equation} \quad (2)$$

Where

$$n1(0-) = N_{C1}\, exp\left(\frac{E_{fn1}(0^-) - Ec(0^-)}{kT}\right)$$ Equation (3)

$$V_{n_1} = \frac{A * T^2}{qN_{c1}}$$ Equation (4)

$$d = \frac{exp(\frac{E_c(0^+)}{kT}}{kT} \int_{E_{min}}^{E_{C(0+)}} exp\,(-\frac{E_x}{kT})\; x\; ...$$

$$... exp(-\frac{4\pi}{h}\int_0^{x_E}\left[2m_n^* Ec(x) - Ex\right]^{1/2} dx)dEx$$ Equation (5)

A similar derivation is being implemented to get the opposite current density of the electron, that is the electrons for another materials and it gives,

$$J_{n2}(0^+) = -qVn_2(1+d)n_2(0^+)$$ Equation (6)

Where

$$n_2(0^+) = N_{c2}\, exp\left(\frac{E_{fn1}(0^+) - Ec(0^+)}{kT}\right)$$ Equation (7)

$$V_{n_2} = \frac{A * T^2}{qN_{c2}}$$ Equation (8)

From Equation above, $V_{n1,2}$ is the mean electron thermal velocity, the effective density of states in the conduction band in each region is denote as $N_{c1,2}$, $n_{1(0-)}$ and $n_{2(0+)}$ are the electron densities at each side of hetero interface, *k* is the Boltzmann constant, T is the temperature , A* is the effective Richardson constant for electrons , *d* is the tunneling probability, $E_{fn1,2}$ represents electrons quasi fermi level in each semiconductor region and $E_c(0^+)$ and $E_c(0^-)$ is the conduction band energy for each materials of GaAs and AlAs. By adding the net electron current density at both side of hetero interface that constitutes of two materials; GaAs and AlAs, the Equation will be as below.

$$Jni = -qV_{n1}\,(1+d)n_1(0^-)x\ldots$$

$$\ldots exp\left(-\frac{\Delta Ec}{kT}\right) + qVn_2\,(1+d)n_2(0^+)$$ Equation (9)

From the Equation 9, the parameter *d* that indicate the tunneling mechanism is being considered in the formulation of current density across the heterojunction (Equation 9). This parameter calculate the probability of electron transmission across heterojunction, thus made the transportation of electron using this formula is actually using the concept of thermionic field emission. If the tunneling mechanism is being neglected, $(T\,(Ex)) = 0$ and thus *d* is equal to zero, then the equation of the current flow will become thermionic emission current. In short, the Equation 9 will be used at the heterointerface of the structure. However, drift diffusion numerical modelling is being applied where the material composition is remaining constant. Moreover, although the tunneling mechanism seems to be evaluated only at the barrier, but it is being evaluated based on the overall conduction band profile at each bias. This implementation can be observed in the COMSOL simulation. By using the mathematical representation for tunneling mechanism at the hetero junction added with the drift diffusion formulation, the two different transport of current that incorporate at the junction can be easily being solved. Apart from that, the recombination-generation process can also be evaluated throughout the whole structure of semiconductors.

NUMERICAL MODELLING: DRIFT DIFFUSION CURRENT TRANSPORT

Drift diffusion model are being used at the remaining structure of the semiconductor. The drift current can be represented from the movement of carriers in certain direction due to the external electrical applied to the structure, whereas the diffusion current is the current that formed from the movement of carriers from higher concentration to a lower concentration. The current applied from external electric and the current movement based on the concentration will then being summed up to get the final current in the remaining structure of semiconductor. Although this study will be focusing on the thermionic field emission and thermionic emission that contribute to the I-V characteristics, it is also significant to know the numerical modelling of drift diffusion model because the material parameters that being used in the asymmetric spacer tunnel diode will being calculated in terms of motion of electrons throughout the whole structure of the ASPAT diode. Based on (Yang et al., 1993), the equation of drift diffusion current can be expressed as follows:

$$\frac{d}{dx}(\epsilon\frac{d\Psi}{dx}) = -q(p-n+N_D^+ - N_A^-)$$ Equation (10)

$$\frac{dJn}{dx} = q(R - G) \qquad \text{Equation (11)}$$

$$Jn = -q\mu_n n \frac{d}{dx}(\psi + \psi_n) - kT\mu_n \frac{dn}{dx} \qquad \text{Equation (12)}$$

$$\psi_n = \frac{X(x) - Xr}{q} + \frac{kT}{q}\ln(\frac{N_c(x)}{N_{cr}}) \qquad \text{Equation (13)}$$

From the equation above, electrostatic potential for n doping is denotes as ψ ,composition dependent band parameters denoted as ψ_n and *X* is the electron affinity. Besides, the parameter values at a reference point in the structure of device is denote as r,μ_n is mobility for electrons, T is temperature and q is charge of electrons. Apart from that, (Yang et al., 1993) also stated that the R which is the rate of recombination also being involved in the electron transportation, and it is assumed to be specified by the Shockley-Hall model as the Equation 14,

$$R = \frac{pn - n_i^2}{\tau_{n0}(p + ni) + \tau_{p0}(n + ni)} \qquad \text{Equation (14)}$$

From the Equation 14, n_i is denote as intrinsic carrier density, the t_{n0} and t_{p0} are the electrons and holes lifetimes, but the solution will be considered for the electrons, as major carrier. The doping concentration for electrons and holes is n and p. Apart from that, the impurities incomplete ionization, $N_D^+ \; and \; N_A^+$ is also being considered by using Equation 15,

$$N_{D=}^{+}\frac{N_D}{1 + \frac{n}{N_c} g_D exp\left(\frac{\Delta E_D}{N_C}\right)} \qquad \text{Equation (15)}$$

$$N_A^- = \frac{N_A}{1 + \frac{P}{N_V} g_A \exp(\frac{\Delta E_A}{kT})} \qquad \text{Equation (16)}$$

From the Equation 15 and 16 that have been mentioned by (Yang et al., 1993), the acceptor and donor impurity are denotes as N_A and N_D , N_v is the effective density of states in valence band, N_c is the effective density of states in conduction band, k and T is the Boltzmann constant and temperature, p and n is the hole and electron doping concentration, g_D is the ground state degeneracy factors of the donor which consist the value of 2 and g_A is the ground state degeneracy factor of acceptor which consists the value of 4 and lastly, the donor and acceptor activation energy are denotes as ΔE_D and ΔE_A. Acceptor activation energy which is ΔE_A is considered as 0.026eV while the donor activation energy , ΔE_D which is 0.005eV in GaAs. In GaAs, the formulation for the energy band gap at the *T (gamma)* point and the low field mobilities of electrons are expressed as Equation 18 that have been stated by (Yang et al., 1993). From Equation 18, the electron lifetime is μ_n.

$$E_{gf} = 1.519 - 5.405x10^{-4}\frac{T^2}{(T + 204)}\, eV$$

Equation (17)

$$\mu_n = \frac{7200}{[1 + 5.51x10^{-17}(N_D + N_A)]^{0.233}}\, x \left(\frac{300}{T}\right)^{2.3} cm^2/Vs$$

Equation (18)

RESULTS AND DISCUSSION

DC ANALYSIS OF GAAS/ALAS ASYMMETRIC SPACER TUNNEL DIODE

The I-V characteristics was measured at 300 K with the bias range from -1.2 V to -0.01 V for the reverse bias and the value also being taken from 0.05 V to 0.25 V for forward bias. The voltage value is not being taken at zero voltage. This is because, zero voltage do not consume any value, and hence the simulator cannot compute the modelling of the I-V characteristics. However, theoretically, there will have a very minimum current value at zero voltage, thus makes the device to become a zero-voltage switching device. The simulated I-V characteristics of the epitaxial layer of ASPAT diode in COMSOL is shown in Figure 4, the I-V characteristics of ASPAT that have been reported in SILVACO is shown in Figure 5, the log (I)-V characteristics of ASPAT is shown in Figure 6 below.

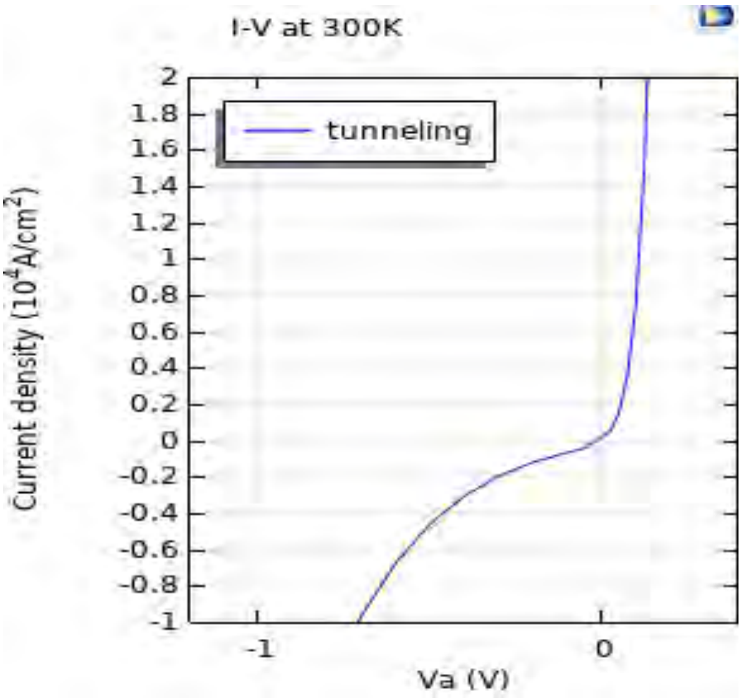


Figure 4: The I-V characteristics of GaAs/AlAs ASPAT diode

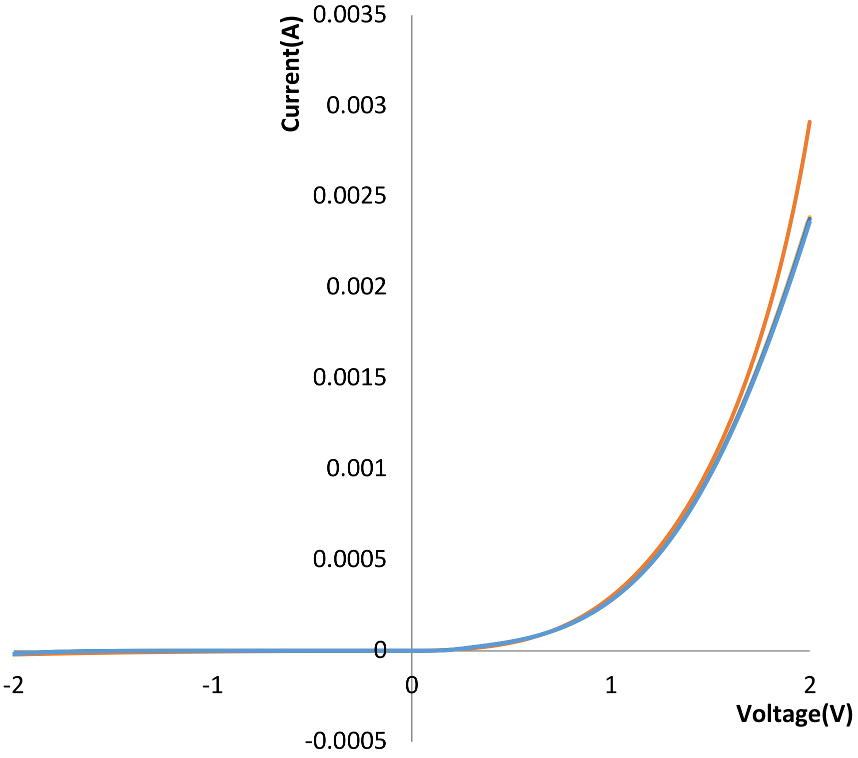


Figure 5: The reported I-V characteristics of ASPAT in SILVACO

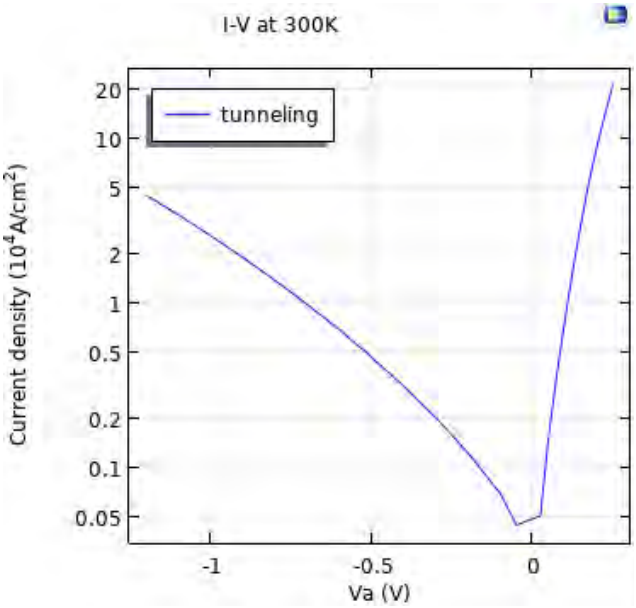


Figure 6: The log(I)-V characteristics of GaAs/AlAs ASPAT diode in COMSOL

Theoretically, the asymmetry spacer in the structure of the ASPAT diode will lead to the asymmetric current - voltage characteristics. This condition can be observed in the physical modelling and the I-V characteristics that have been produced in COMSOL (Figure 4). The asymmetric I-V characteristics that occur can be described from the effect of voltage bias applied towards the band diagram along with the phenomena of thermionic emission current and thermionic field emission current (tunneling current) across the hetero junction. The active structure of the device consists of GaAs (spacer 1), AlAs (barrier) and the GaAs (spacer 2). The dimension of the spacer 1 need to have a large dimension compared to spacer 2 while the barrier needs to maintain with a thinner width. This reason can be explained from the Figure 7 , that previously being stated by (Ariffin, 2019).

Figure 7 above illustrates the ASPAT conduction band profile and how the changes of voltage lead the band banding and the formation of I-V characteristics. The red line, green line and black line are the band bending behavior under forward bias (red line), no bias (black line) and reverse bias (green line). When the asymmetric spacer tunnel diode is being applied with the forward bias (red line), the current will be injected to the device from spacer 1 to the AlAs and end at spacer 2. Here, the band diagram will be stretched downwards and the potential (height) of the barrier will be reduced, as being shown in Figure 8. Another observation is, the electron will also form the small triangular well known as accumulation region at the band diagram in spacer 1, before the electron can tunnel the AlAs. There also will be two types of current transport at the heterojunction during forward bias which is the transport of current due to the thermionic field emission (tunneling current) and the current that happen due to the thermionic emission.

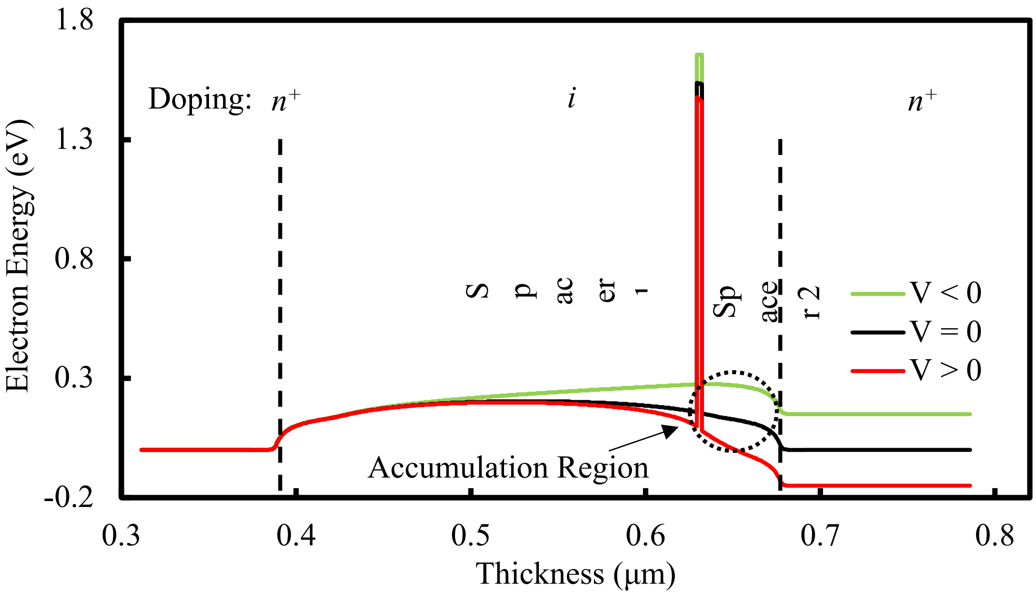


Figure 7: Conduction of Band Profile of ASPAT diode under bias

Based on (Latreche, 2019) thermionic emission current, the electron will jump the barrier (AlAs), while, in thermionic field emission current, the electron will tunnel from GaAs to AlAs. By contrast, the opposite trend can be noted when a reverse bias is applied. In comparison to the increment of the potential barrier during the forward bias, the reverse bias will make the potential bias increases, as being shown in Figure 9.

Most of these voltages drop across the thick intrinsic spacer region and cause only a small number of electrons to reach the barrier under reverse bias conditions. This led to only one type of current can flow under zero voltage (reverse bias), which is the thermionic emission and results a very slow rise in the reverse current bias compared to forward bias, which is the reason for the asymmetric I-V characteristics between forward and reverse biases. From these conditions due to the voltage effects towards band banding, the I-V characteristics in Figure 4 shows an immediate rise in forward bias compared to the reverse bias.

Apart from that, when the I-V characteristics of ASPAT in COMSOL is being compared with the I-V characteristics of ASPAT that have been reported in SILVACO, there is a slight difference in terms of the steepness of the current at the forward and reverse bias, as being shown in Figure 5. The I-V characteristics of ASPAT in COMSOL has an immediate leakage current compared with ASPAT that being modelled in SILVACO This is because of the effect of the doping concentration at the barrier.

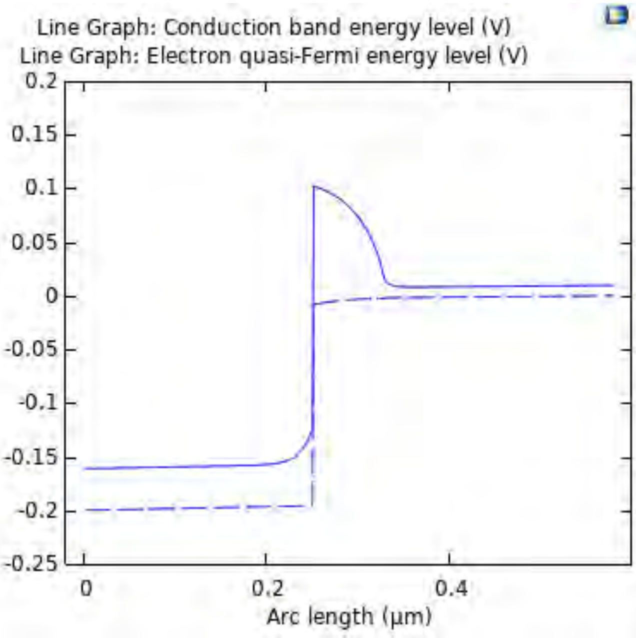


Figure 8: The Effect of Forward Bias to The Potential Barrier (0.2 V)

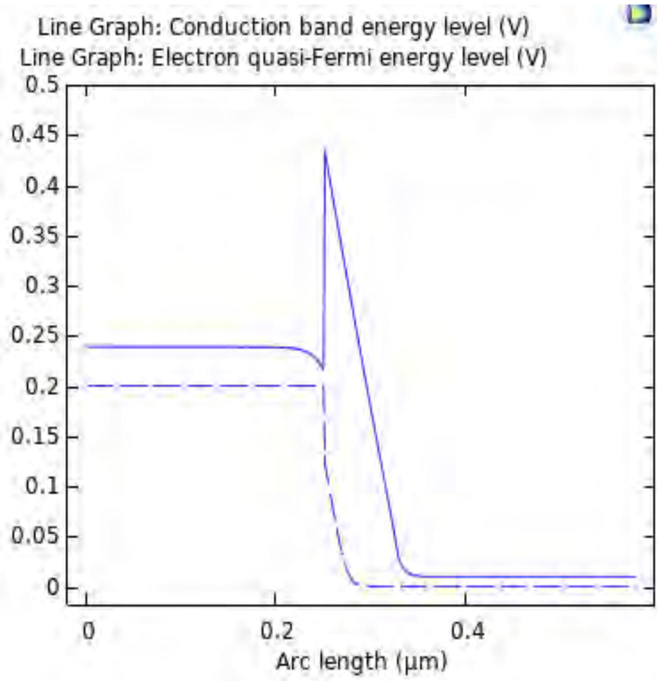


Figure 9: The Effect f Reverse Bias To The Potential Barrier (-0.2 V)

Based on (Yang et al., 1993), the effect of the doping concentration at the barrier. They applied different doping concentration at the barrier and performed the analysis at gives significant effects to the formation of I-V characteristics. In their research, a significant contribution by tunneling is found at higher doping densities at forward bias and the enhancement of current is large at the reverse bias. This is because, the high doping concentration at the barrier makes the barrier becomes thinner. When the barrier thickness is reduced, the probability of the electron to tunnel across the AlAs becomes higher. However, based on Syme et al. (1991) the physical modelling of ASPAT in SILVACO is using zero concentration at the barrier, hence, the enhancement of the current during forward and reverse bias is smaller compared to the physical modelling in COMSOL, that used a high concentration. Besides, based on Figure 6, the graph shows that the zero turn on bias is approaching to the exactly zero value. It is observed for not being accurately measured at zero value due to the limited of construction in simulator. Apart from that, another important theory that need to be noted is, the discontinuity in the fermi level that happen at the interface also indicate that the current transport across the hetero junction is being limited by thermionic emission and thermionic field emission rather than the by using the drift diffusion transport .

CONCLUSIONS

A physical modelling of GaAs/AlAs single barrier asymmetric spacer tunnel diode had been developed in COMSOL Multiphysics. By considering the numerical modelling of thermionic field emission and drift diffusion current across the structure of ASPAT, the current can be calculated when a voltage biased being applied across the structure of the device. There are two unique characteristics that being observed through out the physical modelling of ASPAT, that is the leakage current and zero turn on bias. These characteristics have been produced through out the physical modelling in COMSOL Multiphysics and it is approaching and nearly reciprocate with the characteristics of ASPAT in SILVACO. Therefor, a future adjustment on physical modelling of asymmetric spacer tunnel diode should be taken for optimization of I-V characteristics.

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