Transmittances of an Electron through a Heterostructure Nanometer-Thick Trapezoidal Barrier Grown on an Anisotropic Material for Energy Higher than Potential Barrier

Lilik Hasanah[1)], Khairurrijal, Mikrajuddin Abdullah, Toto Winata, and Sukirno

Department of Physics, Institut Teknologi Bandung, Jalan Ganesha 10, Bandung 40132

Abstract

Effective-mass equation including off-diagonal effective-mass tensor elements has been solved in deriving transmittances of an electron incident on a heterostructure potential with nanometer-thick trapezoidal barrier grown on anisotropic materials. The boundary condition for an electron wave function (under the effective-mass approximation) at the heterostructure anisotropic junction is suggested and included in the calculation. The analytic expression has been applied to the Si(110)/$Si_{0.5}Ge_{0.5}$/Si(110) heterostructure, in which the SiGe barrier thickness is several nanometers. It was assumed that the direction of propagation of the electrons makes an arbitrary angle with respect to the interfaces of the heterostructure and the effective mass of the electron is position dependent. The transmittance has been calculated for above the barrier height with varying the applied voltage to the barrier. The electron incident energy and the bias voltages given to barrier potential influence the transmittance value. The transmittances depend on the valley where the electron belongs and it is not symmetric with respect to the incidence angle but the maximum transmittances not depend on the valley. The maximum transmittance depends on the bias voltage.

[1] On leave from Jurusan Fisika, FPMIPA, Universitas Pendidikan Indonesia, Bandung

Key-words: Anisotropic material, heterostructure, nanometer-thick barrier, transmittance

1. Introduction

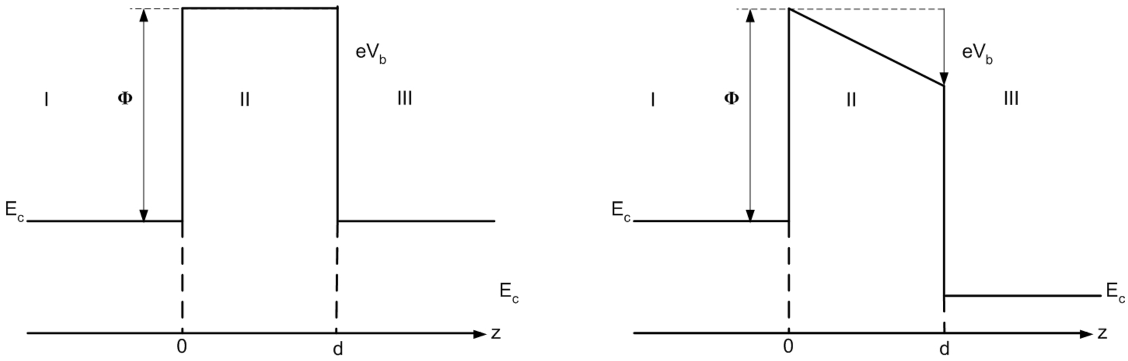
Since last half century, the tunneling phenomenon through a potential barrier is still of interest in the study of quantum transport in heterostructures. Paranjape studied transmission coefficient of an electron in an isotropic heterostructure with different effective masses [1]. Kim and Lee derived the transmission coefficient of an electron tunneling through a barrier of an anisotropic heterostructure by solving the effective-mass equation including off-diagonal effective-mass tensor elements [2],[3]. Previous, we have reported the electron transmittances if bias voltage applied to the potential barrier in which the square barrier becomes trapezoidal one for the electron incident energy lower than potential barrier [4],[5],[6]. In this paper, we report the derivation and the calculation of the transmittance of an electron through a heterostructure with a nanometer-thick trapezoidal barrier grown on an anisotropic material, including the effect of applied voltage to the barrier if the electron incident energy higher than potential barrier.

2. Theoretical Model

The conduction band energy diagram of a heterostructure is shown in Fig 1 with the potential profile is expressed as :

$$V(z)=\begin{cases} 0 & \text{for} \quad z \le 0 \\ \Phi - \dfrac{eV_b}{d} z & \text{for} \quad 0 < z < d \\ -eV_b & \text{for} \quad z \ge d. \end{cases} \qquad (1)$$

Here, the barrier width and height are d and Φ, respectively. The voltage applied to the barrier is V_b with e is the electronic charge. The electron is incident from region I to the potential barrier (region II), in which the material of the region I is the same as that of the region III.



(a) (b)

Figure1. The potential profile of a heterostructure without a bias voltage (a) and with the application of a voltage to the barrier (b)

The Hamiltonian for general anisotropic materials is [2]

$$H = \frac{1}{2m_o}\mathbf{p}^T \alpha(\mathbf{r})\mathbf{p} + V(\mathbf{r}), \tag{2}$$

where m_o is the free electron mass, $\mathbf{p}$ is the momentum vector, $\left(\frac{1}{m_o}\right)\alpha(\mathbf{r})$ is the inverse effective-mass tensor and $V(\mathbf{r})$ is the potential energy. The effective mass of the electron and potential are dependent only on the z direction. The wave function of the effective-mass equation with the Hamiltonian in Eq. (2) is given as [2]:

$$\psi(\mathbf{r}) = \varphi(z)\exp(-i\gamma z)\exp(i(k_x x + k_y y)), \tag{3}$$

and $\gamma = \dfrac{k_x \alpha_{xz} + k_y \alpha_{yz}}{\alpha_{zz}}$ (4)

is wave number parallel to the interface.

By employing the separation variable to Eq. (2), it is easily found that $\varphi(z)$ satisfies the one dimensional Schrödinger-like equation:

$$-\frac{\hbar^2}{2m_o}\alpha_{zz,l}\frac{\partial^2\varphi(z)}{\partial z^2} + V(z)\varphi(z) = E_z\varphi(z)\,, \tag{5}$$

where $\hbar$ is the reduced Planck constant, the subscript l in $\alpha_{zz,l}$ denotes each region in Fig. 1 and electron energy in z direction written as :

$$E_z = E - \frac{\hbar^2}{2m_o}\sum_{i,j\in\{x,y\}}\beta_{ij}k_i k_j\,. \tag{6}$$

Here,

$$E = \sum_{i,j\in\{x,y,z\}}\frac{\hbar^2}{2m_o}\alpha_{ij,1}k_i k_j \tag{7}$$

is the electron total energy,

$$\beta_{ij} = \alpha_{ij} - \frac{\alpha_{iz}\alpha_{zj}}{\alpha_{zz}}\,, \tag{8}$$

and α_{ij} is the effective mass tensor element.

The time-independent electron wave function in each region is therefore written as

$$\psi_1(\vec{r}) = (Ae^{ik_1z} + Be^{-ik_1z})e^{-(i\gamma_1 z)}e^{-(ik_x x + ik_y y)}\,, \qquad \text{for } z \le 0, \tag{9}$$

$$\psi_2(\vec{r}) = (Ce^{-\int_0^z k_2(z)dz} + De^{\int_0^z k_2(z)dz})e^{-(i\gamma_2 z)}e^{-(ik_x x + ik_y y)}\,, \qquad \text{for } 0 < z < d, \tag{10}$$

$$\psi_3(\vec{r}) = Fe^{ik_3z}e^{-(i\gamma_1 z)}e^{-(ik_x x + ik_y y)}\,. \qquad \text{for } z \ge d. \tag{11}$$

The incident wave $A\exp(ik_1z)$ has the wave number k_1 which is given as

$$k_1 = \left\{ \frac{2m_o E_z}{\hbar^2} \frac{1}{\alpha_{zz,1}} \right\}^{1/2}, \tag{12}$$

The wave numbers $k_2(z)$ and k_3 are expressed, respectively, as follows

$$k_2(z) = \left\{ \frac{2m_0}{\hbar^2} \frac{1}{\alpha_{zz,2}} (\Phi - e\frac{V_b}{d} z) - \frac{\alpha_{zz,1}}{\alpha_{zz,2}} k_1^2 - \frac{1}{\alpha_{zz,2}} \sum_{i,j\in(x,y)} (\beta_{ij,1} - \beta_{ij,2}) k_i k_j \right\}^{1/2}, \tag{13}$$

and

$$k_3 = \left\{ \frac{2m_o\left(E_z + eV_b\right)}{\hbar^2} \frac{1}{\alpha_{zz,1}} \right\}^{1/2}. \tag{14}$$

By applying the boundary conditions at z = 0 dan z = d, which are written as follows [3]:

$$\psi_I(z = 0^-) = \psi_2(z = 0^+), \tag{15a}$$

$$\frac{1}{m_o}\left[\alpha_{zx,I}\frac{d\psi_1}{dz} + \alpha_{zy,I}\frac{d\psi_1}{dz} + \alpha_{zz,I}\frac{d\psi_1}{dz}\right]_{z=0^-}$$

$$= \frac{1}{m_o}\left[\alpha_{zx,2}\frac{d\psi_2}{dz} + \alpha_{zy,2}\frac{d\psi_2}{dz} + \alpha_{zz,2}\frac{d\psi_2}{dz}\right]_{z=0^+}, \tag{15b}$$

$$\psi_2(z = d^-) = \psi_3(z = d^+), \tag{15c}$$

$$\frac{1}{m_o}\left[\alpha_{zx,2}\frac{d\psi_2}{dz} + \alpha_{zy,2}\frac{d\psi_2}{dz} + \alpha_{zz,2}\frac{d\psi_2}{dz}\right]_{z=d^-}$$

$$= \frac{1}{m_o}\left[\alpha_{zx,1}\frac{d\psi_3}{dz} + \alpha_{zy,1}\frac{d\psi_3}{dz} + \alpha_{zz,1}\frac{d\psi_3}{dz}\right]_{z=d^+}, \tag{15d}$$

we obtain the transmission amplitude T_a which is defined as

$$T_a = \frac{F}{A} = G\exp(i\phi). \tag{16}$$

Here,

$$G = \frac{2k_1 k'^d_2}{(P'^2 \sin^2(u') + Q'^2 \cos^2(u'))^{1/2}} \tag{17}$$

is the magnitude and

$$\phi = \left[\tan^{-1}\left(\frac{P'}{Q'}\right)\tan(u')\right] - k_3 d + (\gamma_1 - \gamma_2)d \tag{18}$$

is the phase of T_a,

$$P' = \left(\frac{\alpha_{zz,1}}{\alpha_{zz,2}} k_1 k_3 + \frac{\alpha_{zz,2}}{\alpha_{zz,1}} k'^0_2\, k'^d_2\right) \quad , \tag{19}$$

$$Q' = (k_3 k'^0_2 + k_1 k'^d_2), \tag{20}$$

$$k'^0_2 = k'_2\,(z = 0), \tag{21}$$

$$k'^d_2 = k'_2\,(z = d), \tag{22}$$

$$u' = \int_0^d k'_2\,(z) dz, \tag{23}$$

and

$$k'^2_2 = -k^2_2 . \tag{24}$$

3.Results and Discussion

The model used in the numerical calculation is shown in Fig. 1 with a potential barrier is a strained $Si_{0.5}Ge_{0.5}$ potential barrier grown on Si (110). The width of the barrier d is 50 Å and the band discontinuity Φ is taken as 216 meV [2].

There are four equivalent valleys in the conduction bands of Si(110) and strained $Si_{0.5}Ge_{0.5}$. The effective mass tensor elements of these four valleys are not the same.

There are two groups of valleys in Si(110) and $Si_{0.5}Ge_{0.5}$. The inverse effective inverse tensor used in Eq. (2) are related to the tensor elements α_{ij} shown in Table 1 [2]. In Table 1, we see that one group (valley 1) has positive α_{yz}, while another one (valley 2) has negative α_{yz}[3]. We denote the group that has positive α_{yz} as valley 1 and the other as valley 2. Therefore, the calculated results depend on the group which electron belongs.

Table1. Tensor elements (α_{ij}) used in the numerical calculation.

Valley	Region I dan III (Si [110])	Region II ($Si_{0,5}Ge_{0,5}$)
1	5.26 0 0 0 3.14 2.12 0 2.12 3.14	6.45 0 0 0 4.56 2.74 0 2.74 4.56
2	5.26 0 0 0 3.14 -2.12 0 -2.12 3.14	6.45 0 0 0 4.56 -2.74 0 -2.74 4.56

Figure 3 shows the chosen coordinate system. We take the position where the electron hits the barrier as the origin of the coordinate system. In the spherical coordinate system, Eq. (7) becomes

$$\begin{aligned} E = \frac{\hbar^2}{2m_o}\Big\{ & \alpha_{xx1}k^2\sin^2\theta\cos^2\varphi + \alpha_{yy1}k^2\sin^2\theta\sin^2\varphi + \alpha_{zz1}k^2\cos^2\theta \\ & + 2\big(\alpha_{xy1}k^2\sin^2\theta\cos\varphi\sin\varphi + \alpha_{yz1}k^2\sin^2\theta\cos\theta\sin\varphi \\ & + \alpha_{zx1}k^2\sin^2\theta\cos\theta\cos\varphi\big)\Big\} \end{aligned} \quad . \tag{25}$$

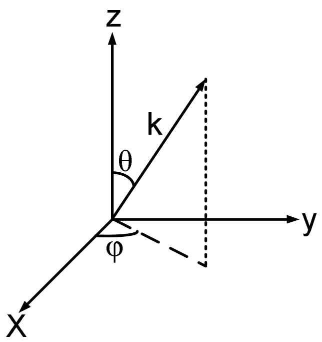


Figure.3. The coordinate system used in the analysis

We calculated the transmission coefficient for the angle of incidence for **k** (the wave vector of incident electron) varying from -90^o to 90^o with incident energies of 250meV, 500meV, and 1000meV with varying the applied voltage from 5 mV to 216 mV. The incident angles are θ and φ, but we fix φ to π/2 for simplicity and change only θ.

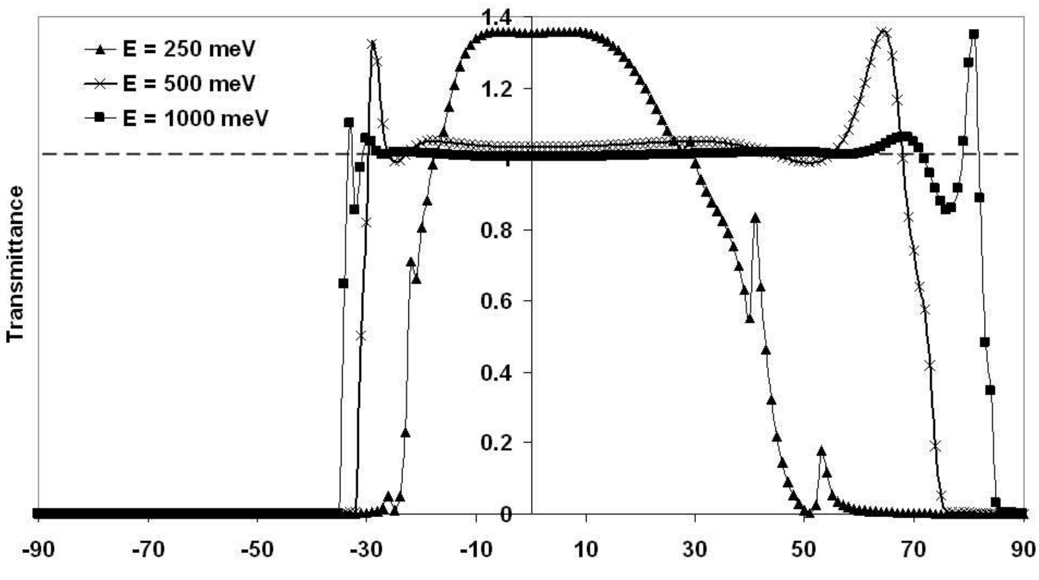


Figure 4. The transmittance to incident angle for the incident angle varying from -90^o to 90^o with incident energy of 250 meV, 500 meV and 1000 meV with applied voltage of 50 mV for valley 1.

The transmittance as a function of incident angle for incident energy of of 250 meV, 500 meV and 1000 meV with applied voltage of 50 mV for valley 1 is shown in Fig. 4. For all incident energy, we can see the highest transmittances are about 1.4.

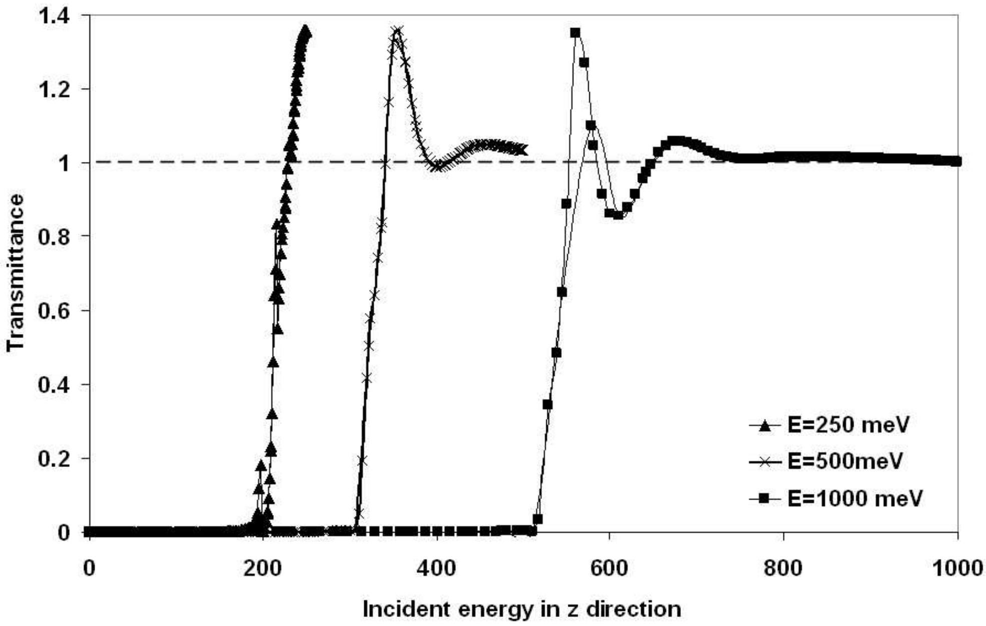
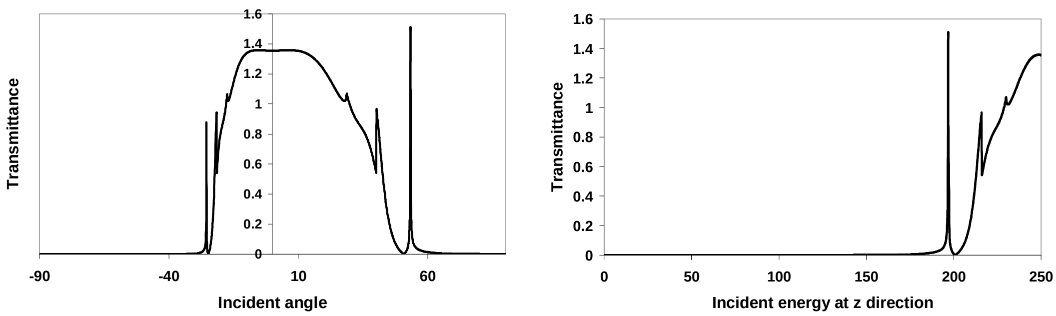


Figure 5. The transmittance to incident energy in z direction for the incident angle varying from -90^o to 90^o with incident energy of 250 meV, 500 meV and 1000 meV with applied voltage of 50 mV for valley 1.

In Fig. 5, transmittance plot to incident energy in z direction (E_z). For all incident energies, after transmittances reach the highest transmittance, the transmittance will decrease and oscillation at value around 1. For the incident energy of 250meV, the highest transmittance occurs at about normal incidence shown at Fig. 4. At this angle, the incident energy in z direction, E_z, is biggest shown in Fig. 5. But for the incident energy 500meV, the highest transmittance occurs at incident angle -30^o and 70^o but at incident angle -30^o to 70^o the transmittance is around 1 shown in Fig.4. This caused by at incident angle -30^o and 70^o the incident energy in z direction, E_z, is about 350meV which give the maximum transmittance and E_z at $-30^o<\theta<70^o$ is bigger than 350meV where the transmittances decrease and oscillation at value about 1 shown in Fig.5. In Fig. 5, it is seen effect of incident energy to the transmittances value that is the same transmittances value not given from the same E_z. For the same transmittances value, the value of E_z increase as the incident energy increase. It is cause by the same E_z from different incident energy will give different the wave numbers in region II, $k_2(z)$. E_z and $k_2(z)$ value depends on incident energy and angle. For incident energy 250 meV, if we plot the graph for the difference small angle, we will get the transmittance to incident angle like showed in Fig. 6. Fig 6(a) shows that the transmittance at incident angle about 55^o is higher than at normal incidence and it is happen at E_z about 200 meV like showed in Fig 6(b).



(a) (b)

Figure 6. The transmittance to incident angle (a) and Ez (b) for incident energy 250 meV

In Fig.7 we fix the incident energy to 500 meV and applied voltage of 5 mV, 50 mV, 108 mV and 216 mV for valley 1. It is found that the maximum transmittance increase with increased the applied voltage. The incident energy in z direction, E_z, which makes transmittance maximum decrease with increased the applied voltage. It can see that for the same E_z the transmittances value will increase as the applied voltage increased. From this, we can say that the applied voltage given to potential barrier will make the electron easier to tunneling the potential barrier. For all the incident energy, transmittances will increase if the incident energy is increased and after reaching the highest transmittance, transmittance will decrease and oscillating at value 1.

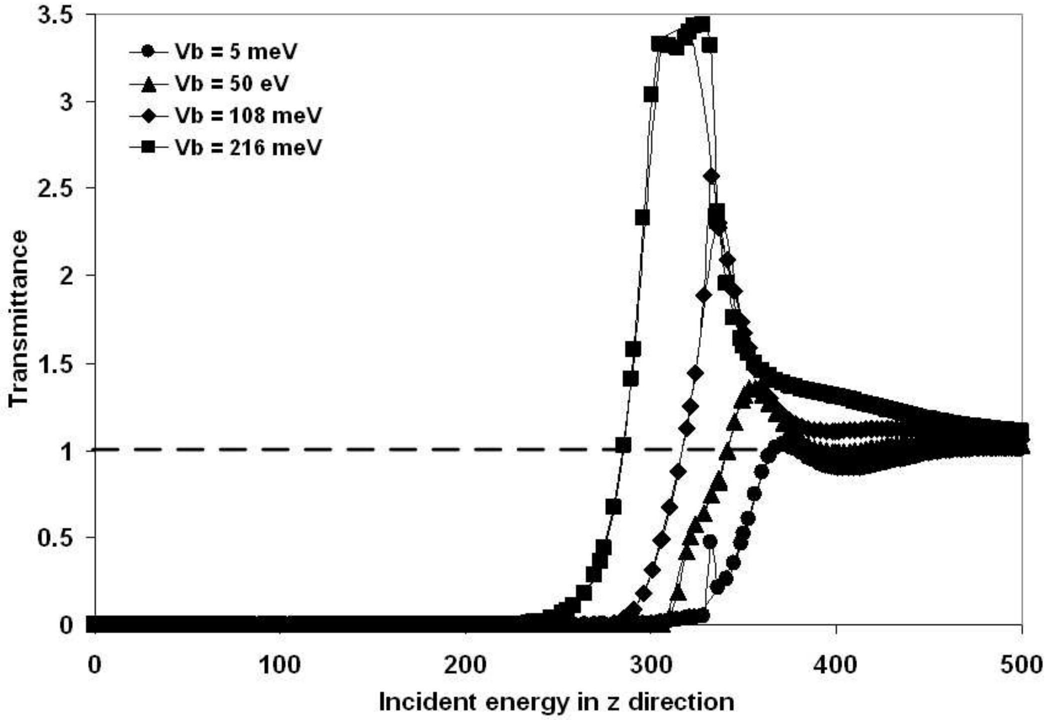


Figure 7. The transmittance to incident energy in z direction for the incident angle varying from -90^o to 90^o with incident energy 500 meV and applied voltage of 5 mV, 50 mV, 108 mV and 216 mV for valley 1.

If we plot transmittances to incident angle, we can see that the maximum transmittance occurs at incident angle about -30^o and 70^o but at incident angle -30^o to 70^o the transmittance is around 1 as shown in Fig. 8. It is because the E_z value depends on incident angle and we get the E_z value like shown in Fig.7. In Fig 9, we fix the applied voltage to 216 mV and the incident energy to 1000meV. The highest transmittance happen at E_z about 500meV and after reaching the maximum transmittance, the transmittance is stable at value about 1 with increasing the incident energy.

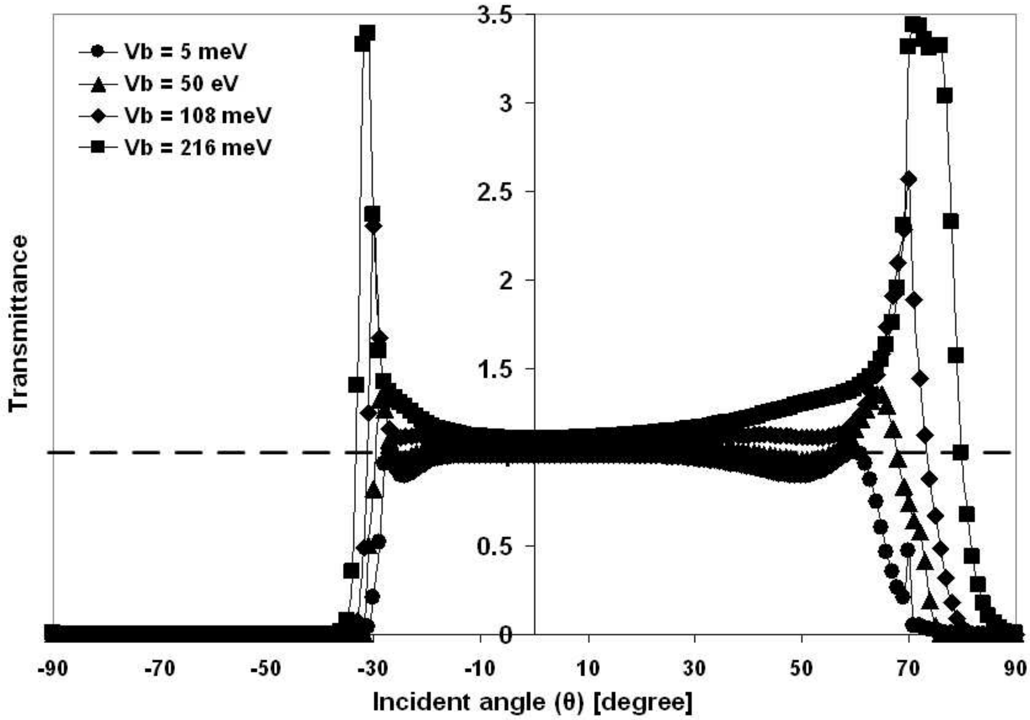


Figure 8. The transmittance to incident angle for the incident angle varying from -90^o to 90^o with incident energy 500 meV and applied voltage of 5 mV, 50 mV, 108 mV and 216 mV for valley 1.

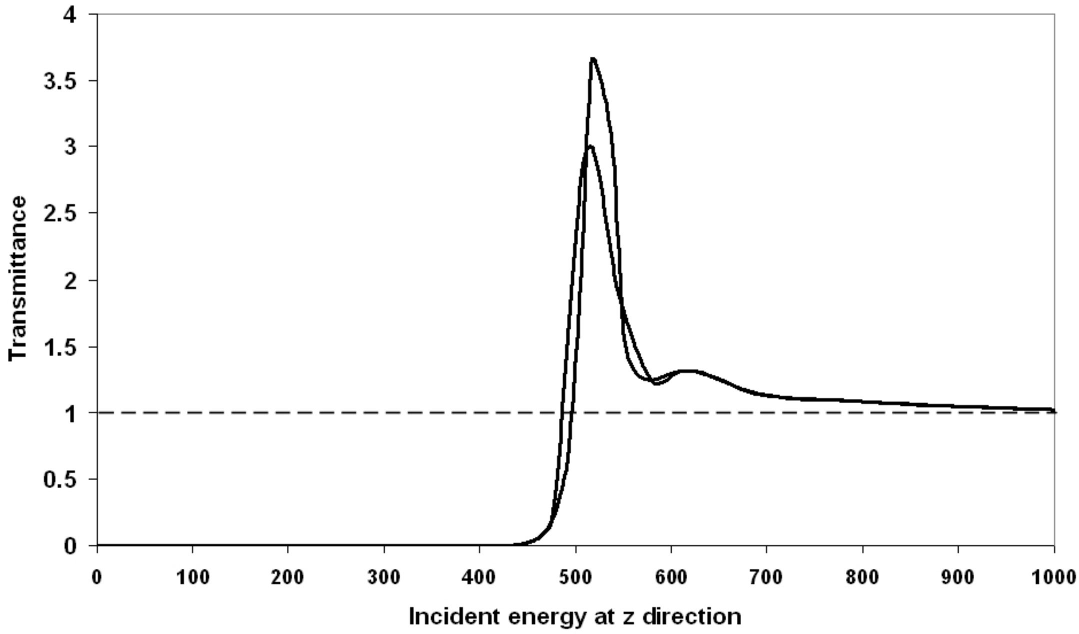
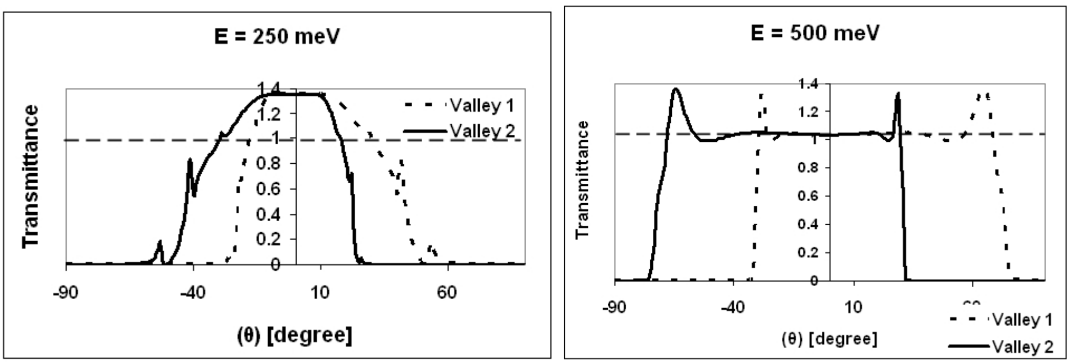


Figure 9. The transmittance to incident energy in z with incident energy 1000 meV and applied voltage of 216 mV for valley 1.



(a) (b)

Figure 10. The transmittance to incident angle for the incident angle varying from -90^o to 90^o with incident energy of (a) 250 meV and (b) 500 meV with applied voltage of 50 mV for valley 1 and valley 2.

Fig. 10 shown the transmittance for incident energy of 250meV and 500meV with applied voltage of 50 mV for valley 1 and valley 2. For valley 1 and valley 2, for the same incident energy, the maximum transmittances will have the same value but the shape of transmittances graph like mirror. The sign ± corresponds to valley 1 and 2, respectively. This difference in direction also indicates the anisotropy of the material. It is due to the fact that the motion in the x and y directions is not independent of that in the z direction, but they are mutually coupled by the off-diagonal effective-mass tensors elements[2]. For incident energy of 250meV, it is found that electron in the valley 1 and valley 2 have the highest transmission coefficient at about normal incidence. We also see that, in all valleys, the transmission coefficient is not symmetric with the change of sign of incidence angle (θ→-θ), which confirms the anisotropic of the materials [2].

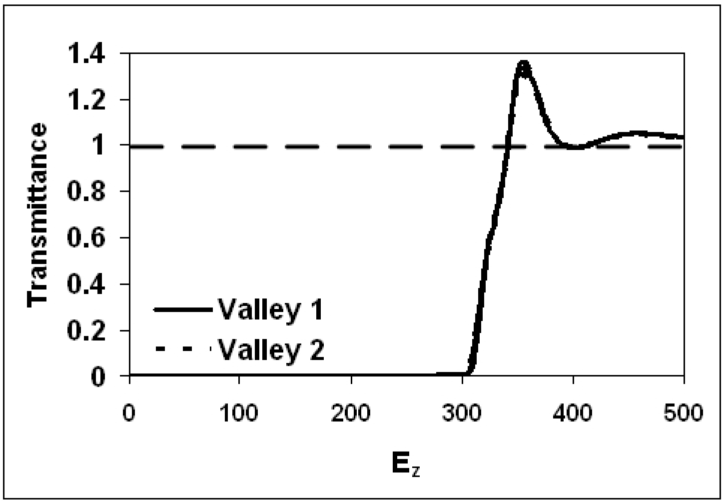


Figure 11. The transmittance to incident energy for the incident angle varying from -90^o to 90^o with incident energy 500meV with applied voltage of 50 mV for valley 1 and valley 2.

For case at Fig. 10 (d) if we plot the transmittance to incident energy in z direction, E_z, we will get graph like Fig.11. It is show the same shape for all valleys. Transmittances at valley 1 and 2 will get the same value when E_z are the same. E_z of valley 1 and 2 will have the same value depend on the incident angle of valley 1 and 2. This indicates that for the same incident energy and applied voltage, the maximum transmittance will be same whatever the valleys.

Conclusion

We have derived an analytical expression of transmittance of an electron through a nanometer-thick trapezoidal barrier grown on anisotropic materials under non-normal incidence. We included the effect of different effective masses at heterojunction interfaces. The boundary conditions for electron wave functions (under the effective-mass approximation) at heterostructure anisotropic junctions are suggested and included in the calculation. The transmittance will decreased after reaching the highest transmittance then stable at value about 1. For the same transmittances value, the value of incident energy at z direction increase as the incident energy increase. In the same incident energy, the maximum transmittance increased with increased the applied voltage to the barrier and for the same E_z the transmittances value will increase as the applied voltage increased. The result shows that the transmittances depend on the valley where the electron belongs and it is not symmetric with respect to the incidence angle but the maximum transmittances not depend on the valley.

Acknowledgment

One of the authors (L.H) would like to thank the Habibie Center for the domestic doctoral scholarship.

References:

[1] V.V. Paranjape: Transmission coefficient and stationary-phase tunneling time of an electron through a heterostructure, *Phys.Rev. B*. Vol 52. No 15, 1995, 10 740-10 743

[2] K.-Y. Kim and B. Lee: Transmission coefficient of an electron through a heterostructure barrier grown on anisotropic materials, *Phys.Rev. B*. Vol 58. No 11, 1998, 6728-6731

[3] K.-Y. Kim and B. Lee: Tunneling time and the post-tunneling position of an electron through a potential barrier in an anisotropic semiconductor, *Superlattice Microstruct*. Vol 24. No 6, 1998, 389-397

[4] L. Hasanah, Khairurrijal, Mikrajudin, T. Winata and Sukirno : Tunneling Time and Transmission Coefficient of An Electron Tunneling Through A Nanometer-Thick Square Barrier in an Anisotropic Heterostructure, Proc. Int. Conf. Applied .Math .(ICAM05), Bandung 22-26 August 2005, CP14.

[5] L. Hasanah, F. A. Noor, Khairrurijal, Mikrajuddin, T. Winata dan Sukirno : Koefisien transmisi elektron yang melalui pemghalang dengan ketebalan nanometer pada heterostruktur anisotropic yang diberi tegangan panjar, Proc. Nas. 3rd Kentingan Physics Forum (KPI), Solo 24 September 2005, 152-154

[6] L. Hasanah, F. A. Noor, Khairrurijal, Mikrajuddin, T. Winata dan Sukirno : Transmission Coefficient of an Electron through a Heterostructure with Nanometer-

Thick Trapezoidal Barrier Grown on an Anisotropic Material, *Proc. ITB Sains & Tek.* Vol. 38 A, No. 1, 2006, pp. 41-50