Electron Transmittance at Si(110)/$Si_{0.5}Ge_{0.5}$/Si(110) Anisotropic Heterostructure with Bias Voltage for Incident Energy Lower than Potential Barrier

Lilik Hasanah[#], Khairurrijal[§], Mikrajuddin Abdullah, Toto Winata, and Sukirno
Physics of Electronic Materials Division, Faculty of Mathematics and Natural Sciences
Institut Teknologi Bandung, Jalan Ganesha 10, Bandung 40132, Indonesia
[#]Jurusan Fisika, FPMIPA, Universitas Pendidikan Indonesia, Jl. Setiabudhi no 229 Bandung 40154
[§]Electronic mail: krijal@fi.itb.ac.id

Abstract

Analytic expressions of transmittance of an electron incident on a heterostructure potential with nanometer-thick trapezoidal barrier grown on anisotropic materials have been derived by solving the effective-mass equation including off-diagonal effective-mass tensor elements. It was assumed that the direction of propagation of the electron makes an arbitrary angle with respect to the interfaces of the heterostructure and the effective mass of the electron is position dependent. The analytic expressions have been applied to the Si(110)/$Si_{0.5}Ge_{0.5}$/Si(110) heterostructure, in which the $Si_{0.5}Ge_{0.5}$ barrier thickness is 5 nm. The transmittance has been calculated for incident energy at z direction below the barrier height with varying the applied voltage to the barrier. There are the direct and the Fowler Nordheim tunneling depending on electron incident energy. The electron incident energy, the bias voltages given to barrier potential and the valley of Si(110)/$Si_{0.5}Ge_{0.5}$/Si(110) influence the transmittance value.

Keywords: *Anisotropic material, heterostructure, nanometer-thick barrier, transmittance*

I. Introduction

Since last half century, the tunneling phenomenon through a heterostructure potential barrier is still of interest in the study of quantum transport in heterostructures. Lee done analysis of the electron tunneling time through a heterostructure barrier including the position-dependent effective-mass effect with adopts wigner's phase time approach [1]. Paranjape studied transmission coefficient of an electron in an isotropic heterostructure with different effective masses [2]. Lee compared a one-dimensional theoretical phase time for electron tunneling with simulations results performed with the software Interquanta [3]. 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 [4],[5]. Khairrurial, et al. derived the electron direct tunneling time through a trapezoidal barrier by employing the Wigner phase time [6]. J. Nanda, et al. studied a computational model based on non-relativistic approach for determination of transmission coefficient, resonant tunneling energies, group velocity, resonant tunneling lifetime and transversal time in multibarrier systems (GaAs/$Al_yGa_{1-y}As$) for energy lower and higher than potential barrier height [7]. Previous, we have calculated the electron transmittances and tunneling time of electron through heterostructure square potential barrier which grown on anisotropic material Si(110)/$Si_{0.7}Ge_{0.3}$/Si(110) [4]. Then we studied theoretically electron transmittance if bias voltage applied to the potential barrier in which the square barrier becomes trapezoidal one for Si(110)/$Si_{0.7}Ge_{0.3}$/Si(110) [5] and Si(110)/$Si_{0.5}Ge_{0.5}$/Si(110) structures [6] with the electron incident energy lower than potential barrier. Here, we report the derivation and the calculation of the transmittance of an electron through an Si(110)/$Si_{0.5}Ge_{0.5}$/Si(110) 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 lower than potential barrier and variation of valley Si(110)/$Si_{0.5}Ge_{0.5}$/Si(110).

II. Theoretical Model

In order to study the behavior of an electron in an anisotropic heterostructure, we must solve the Schrödinger equation

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{1}$$

where

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

H is Hamiltonian, m_o is is the free electron mass, **p** is the momentum vector, $(1/m_o)\alpha$ is the inverse effective-mass tensor and $V(\mathbf{r})$ is the potential energy. Fig. 1 show potential profil at z direction The electron is incident from region I to the potential barrier (region II). The effective mass of the electron is dependent only on the z direction. The wave function of the effective-mass equation with the Hamiltonian in Eq. (2) is given as

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

where

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

$\varphi(z$ satisfies the one dimensional Schrödinger-like equation:

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

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 :

$$E_z = E - \frac{\hbar^2}{2m_o}\sum_{i,j\in\{x,y\}}\beta_{ij}k_ik_j , \quad (6)$$

where the electron total energy and

$$\beta_{ij} = \alpha_{ij} - \frac{\alpha_{iz}\alpha_{zj}}{\alpha_{zz}} , \quad (7)$$

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

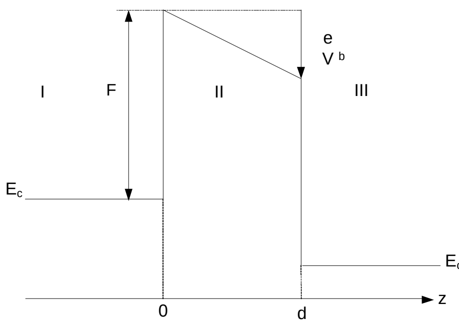

Figure 1. Model used in numerical calculation.

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

$$\Psi_I(z) = (Ae^{ik_1z} + Be^{-ik_1z})e^{-(i\gamma_1 z)}e^{-(ik_xx+ik_yy)} \quad z \le 0, \quad (8)$$

$$\Psi_3(z) = Fe^{ik_3z}e^{-(i\gamma_1 z)}e^{-(ik_xx+ik_yy)} \quad z \ge d, \quad (9)$$

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

$$k_1 = \left\{\frac{2m_oE_z}{\hbar^2}\frac{1}{\alpha_{zz,I}}\right\}^{1/2} , \quad (10)$$

and k_3 are expressed as follows

$$k_3 = \left\{\frac{2m_o\left(E_z + eV_b\right)}{\hbar^2}\frac{1}{\alpha_{zz,I}}\right\}^{1/2} , \quad (11)$$

where Φ is barrier height due to band discontinuity of Si(110) and $Si_{0.5}Ge_{0.5}$ and the voltage applied to the barrier is V_b with e is the electronic charge. By applying the boundary conditions at z = 0 dan z = d, which are written as follows [5]

$$\psi_I(z = 0^-) = \psi_2(z = 0^+) , \quad (12a)$$

$$\frac{1}{m_o}\left[\alpha_{zx,I}\frac{d\psi_1}{dz} + \alpha_{zy,I}\frac{d\psi_1}{dz} + \alpha_{zz,I}\frac{d\psi_1}{dz}\right]_{z=0^-} = \frac{1}{m_o}\left[\alpha_{zx,2}\frac{d\psi_2}{dz} + \alpha_{zy,2}\frac{d\psi_2}{dz} + \alpha_{zz,2}\frac{d\psi_2}{dz}\right]_{z=0^+} , \quad (12b)$$

$$\psi_2(z = d^-) = \psi_3(z = d^+) , \quad (12c)$$

$$\frac{1}{m_o}\left[\alpha_{zx,2}\frac{d\psi_2}{dz} + \alpha_{zy,2}\frac{d\psi_2}{dz} + \alpha_{zz,2}\frac{d\psi_2}{dz}\right]_{z=d^-} = \frac{1}{m_o}\left[\alpha_{zx,1}\frac{d\psi_3}{dz} + \alpha_{zy,1}\frac{d\psi_3}{dz} + \alpha_{zz,1}\frac{d\psi_3}{dz}\right]_{z=d^+} . \quad (12d)$$

we obtain the transmission amplitude T_a which is defined as

$$T_a = G\exp(i\phi) , \quad (13)$$

The transmission coefficient is easily obtained from Eq. (13) by employing the expression

$T = T_a^* T_a$. (14)

III. Results and Discussion

Figures 1 and 2 show that potential barrier $Si_{0.5}Ge_{0.5}$ (region II) grown on Si (110) (region I and III). The barrier width is 50Å band discontinuity is 216 meV [2]. The inverse effective inverse tensor used in this paper is related to the tensor elements α_{ij} shown in Table 1 [4]. In this transmittance calculation, region I and III is valley 2 and region II is valley 1.

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

Valley	Region I and 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 2 shows the chosen coordinate system. We take the position where the electron hits the barrier as the origin of the coordinate system.

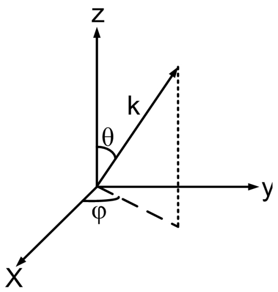

Figure 2. The coordinate system used in the analysis

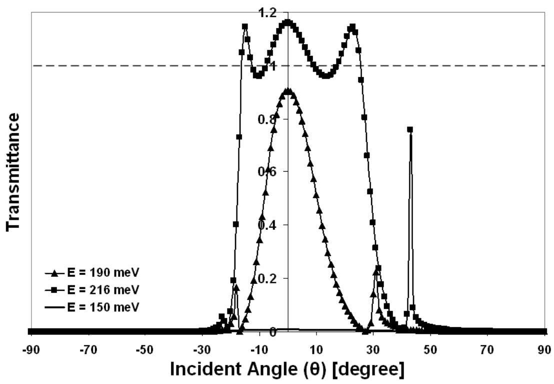

Figure 3. Transmittance as a function of incident angle with incident energies of 150, 190 and 216 meV with applied voltage of 50 mV for valley 1.

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. The incident angles are θ and φ, but we fix φ to π/2 for simplicity and change only θ. The incident angle influences the incident energy at z direction. The incident energies are 150, 190, dan 216 meV and the variation of applied voltage given to potential barrier are 5, 50, 108 and 216 mV. Figure 3 shows transmittance to incident angle for incident energies 150, 190 and 216 meV with bias voltage is 50 mV. It can be seen that the transmittance will increase as the incident electron energy increases because probability of electron to tunnel the barrier will increase if the incident electron energy increased. For the incident energy of 216 meV, there are forbidden energies which incident angles give transmittance values bigger than 1. The forbidden energies happen at incident angle about -20^o to -12^o, -9^o to 10^o and 20^o to 30^o.

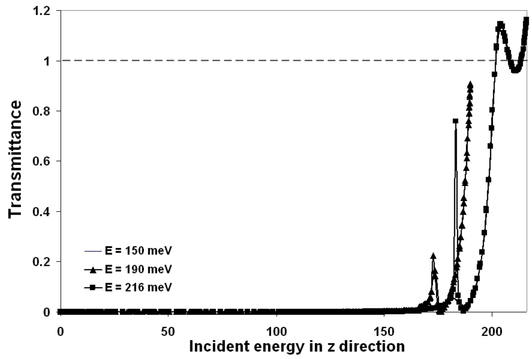

Figure 4. Transmittance as a function of incident energy in z direction for the incident angle varying from -90^o to 90^o with incident energies of 150, 190, and 216 meV with applied voltage of 50 mV.

Plot transmittance to electron incident energy at z direction shown by Fig. 4. We can see that E_z which make the transmittance maximum will increase as the electron incident energy increase. For incident energy 216 meV, the higher transmittance is about 1.15 at E_z value about 200 meV and 216 meV. The transmittance will oscillate at value 1 if E_z value bigger than 216 meV as shown at Fig. 4.

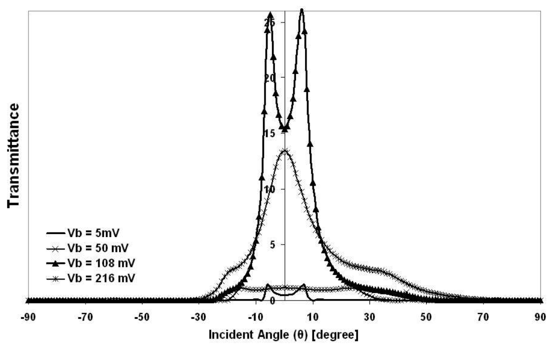

Figure 5. Transmittance for incident angle varying from -90^o to 90^o with incident energies of 216 meV and applied voltages of 5, 50, 108 and 216 mV.

In Fig.5 and 6 we fix the incident energy to 216 meV and applied voltage of 5 mV, 50 mV, 108 mV and 216 mV. Here, we can see that the maximum transmittance at bias voltage 108 mV is higher than at bias voltage 5mV, 50 mV dan 216 mV. For bias voltage given to potential barrier 50 mV, 108 mV and 216 mV forbidden energy happen at incident angle about 25^o to 60^o that is at E_z bigger than 160 meV. Whereas, for bias voltage 50 mV, forbidden energy happen at incident angle -5^o to 10^o that is at E_z bigger than 200 meV. Here, we can see that valley variation at $Si(110)/Si_{0.5}Ge_{0.5}/Si(110)$ influence the probability electron to tunnel potential barrier.

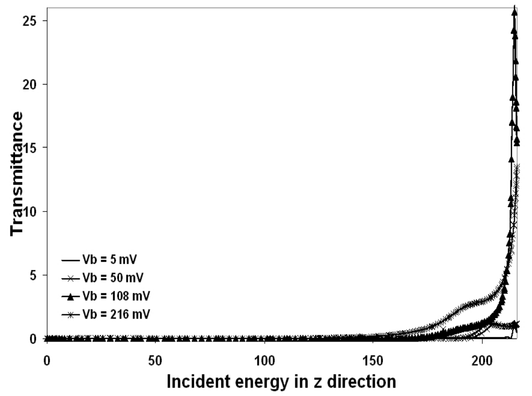

Figure 6. Transmittance as a function of incident energy at z direction with incident energy of 216 meV and applied voltages of 5, 50, 108 and 216 mV.

IV. Conclusion

We have derived an analytical expression of transmission coefficient of an electron through a nanometer-thick trapezoidal barrier grown on anisotropic materials under non-normal incidence. The calculation done for $Si_{0.5}Ge_{0.5}$ potential barrier grown on Si(110). The maximum transmittance influenced by electron incident energy, bias voltage given to potential barrier, and valley variation $Si(110)/Si_{0.5}Ge_{0.5}/Si(110)$. There are some forbidden energies at specific incident angles which make the transmittances value bigger than one.

V. Acknowedgment

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

VI. References

[1] B. Lee : Electron tunneling time through a heterostructure potential barrier, *Superlattice Microstruct.* Vol 14. No 4, 1993, 295-298

[2] 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

[3] B. Lee, W. Lee : Electron tunneling through a potential barrier under non-normal incidence, *Superlattice Microstruct*. Vol 18. No 3, 1998, 177-185

[4] 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

[5] 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

[6] Khairurrijal, F.A. Noor and Sukirno : Electron direct tunneling time in heterostructures with nanometer-thick trapezoidal barriers, *Solid-states electronics*, article in press, 2005

[7] J. Nanda, P.K Mahapatra and C.L. Roy : Transmission coefficient, resonant tunneling lifetime and traversal time in multibarrier semiconductor heterostructure, *Phys.B*, article in press, 2006

[8] 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.

[9] L. Hasanah, F. A. Noor, Khairurrijal, 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

[10] K.-Y. Kim and B. Lee, ”Wigner Function Formulation in Anisotropic Semiconductor Quantum Wells” *Phys.Rev. B*, vol. 64, 115304, 2001.