Transmission Coefficient of an Electron through a Heterostructure with Nanometer-Thick Trapezoidal Barrier Grown on an Anisotropic Material

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Abstract. Transmission coefficient of an electron incident on a heterostructure potential with nanometer-thick trapezoidal barrier grown on anisotropic materials are derived by solving the effective-mass equation including off-diagonal effective-mass tensor elements. The boundary condition for an electron wave function (under the effective-mass approximation) at a heterostructure anisotropic junction is suggested and included in the calculation. The analytic expressions are applied to the Si(110)/$Si_{0.5}Ge_{0.5}$/Si(110) heterostructure, in which the SiGe barrier thickness is several nanometers. It is 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 transmission coefficient is calculated for energy below the barrier height, varying the applied voltage to the barrier. The transmission coefficient depends on the valley where the electron belongs and it is not symmetric with respect to the incidence angle.

Keywords: *Anisotropic material; heterostructure; nanometer-thick barrier; transmission coefficient; tunneling time.*

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]. The effects of different effective masses to the heterostructure were also included but they did not consider the effects of voltage applied to the barrier in which the square barrier becomes trapezoidal one. In this paper, we report the derivation and the calculation of the transmission coefficient of an electron through a heterostructure with a

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Makalah diterima redaksi tanggal 15 Desember 2005, revisi diterima tanggal 29 Maret 2006.

nanometer-thick trapezoidal barrier grown on an anisotropic material, including the effect of applied voltage to the barrier.

2 Theoretical Model

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

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

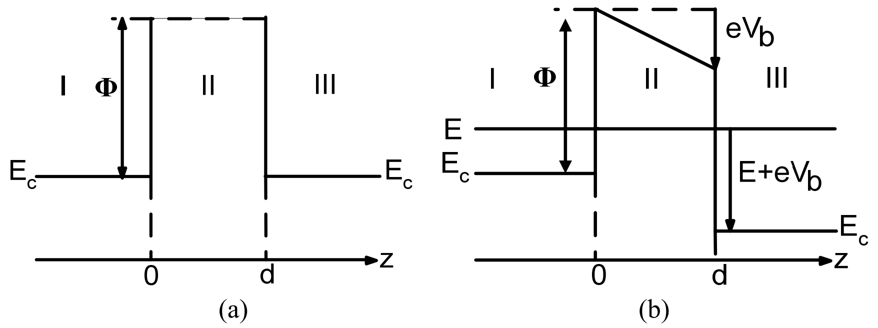

Figure 1 The potential profile of a heterostructure without a bias voltage (a) and with the application of a voltage to the barrier (b).

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.

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, $(1/m_o)\alpha(\mathbf{r})$ 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]:

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

$$\text{and } \gamma = \frac{k_x\alpha_{xz} + k_y\alpha_{yz}}{\alpha_{zz}} \tag{4}$$

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

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

Here,

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

is the 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

$$\psi_1(\vec{r}) = (Ae^{ik_1z} + Be^{-ik_1z})e^{-(i\gamma_1z)}e^{-(ik_xx+ik_yy)}\text{, for } z \le 0, \tag{9}$$

$$\psi_2(\vec{r}) = (Ce^{-\int_0^z k_2(z)dz} + De^{\int_0^z k_2(z)dz})e^{-(i\gamma_2z)}e^{-(ik_xx+ik_yy)}\text{, for } 0 < z < d, \tag{10}$$

$$\psi_3(\vec{r}) = Fe^{ik_3z}e^{-(i\gamma_1z)}e^{-(ik_xx+ik_yy)}\text{, for } z \ge d. \tag{11}$$

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

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

where E_z is smaller than the barrier height Φ. The wave numbers $k_2(z)$ and k_3 are expressed, respectively, as follows

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

and

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

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

$$\psi_I(z = 0^-) = \psi_2(z = 0^+), \quad (15a)$$

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

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

$$\psi_2(z = d^-) = \psi_3(z = d^+), \quad (15c)$$

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

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

we obtain the transmission amplitude T_a which is defined as

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

Here,

$$G = \frac{2k_1 k_2^d}{(P^2 Sinh^2(u) + Q^2 Cosh^2(u))^{\frac{1}{2}}} \quad (17)$$

is the magnitude and

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

is the phase of T_a,

$$P = (\frac{\alpha_{zz,1}}{\alpha_{zz,2}} k_1 k_3 - \frac{\alpha_{zz,2}}{\alpha_{zz,1}} k_2^0 k_2^d), \quad (19)$$

$$Q = (k_3 k_2^0 + k_1 k_2^d), \quad (20)$$

$$k_2^0 = k_2(z=0), \quad (21)$$

$$k_2^d = k_2(z=d), \quad (22)$$

and

$$u = \int_0^d k_2(z) dz . \quad (23)$$

The transmission coefficient is easily obtained from Eq. (16) by employing the expression

$$T = T_a^* T_a. \quad (24)$$

If the voltage applied to the barrier is zero, then $k_2^0 = k_2^d = k_2$, $k_1 = k_3$, and the expressions in Eqs. (17) and (18) will be the same as that given by Lee [2], in which

$$G = \frac{2k_1 k_2}{(P^2 Sinh^2(u) + Q^2 Cosh^2(u))^{1/2}}, \quad (25)$$

$$\phi = \left[\tan^{-1}\left(\frac{P}{Q}\right)\tanh(u)\right] - k_3 d + (\gamma_1 - \gamma_2) d, \quad (26)$$

where

$$P = (\frac{\alpha_{zz,I}}{\alpha_{zz,2}} k_1^2 - \frac{\alpha_{zz,2}}{\alpha_{zz,I}} k_2^2), \quad (27)$$

$$Q = 2k_1 k_2, \quad (28)$$

and

$$u = k_2 d . \quad (29)$$

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 dependent on the group which electron belongs.

Table 1 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	6.45	0	0
	0	3.14	2.12	0	4.56	2.74
	0	2.12	3.14	0	2.74	4.56
2	5.26	0	0	6.45	0	0
	0	3.14	-2.12	0	4.56	-2.74
	0	-2.12	3.14	0	-2.74	4.56

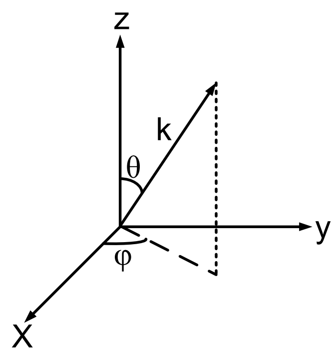

Figure 2 The coordinate system used in the analysis.

Figure 2 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

$$E = \frac{\hbar^2}{2m_o}\left\{\alpha_{xx1}k^2 \sin^2\theta\cos^2\varphi + \alpha_{yy1}k^2 \sin^2\theta\sin^2\varphi + \alpha_{zz1}k^2\cos^2\theta \right.$$
$$+ 2\left(\alpha_{xy1}k^2 \sin^2\theta\cos\varphi\sin\varphi + \alpha_{yz1}k^2\sin^2\theta\cos\theta\sin\varphi \right. \quad . \quad (30)$$
$$\left.\left. + \alpha_{zx1}k^2\sin^2\theta\cos\theta\cos\varphi\right)\right\}$$

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 25 meV, 75 meV and 150 meV and varying the applied voltage from 50 mV to 150 mV. The incident angles are θ and φ, but we fix φ to π/2 for simplicity and change only θ.

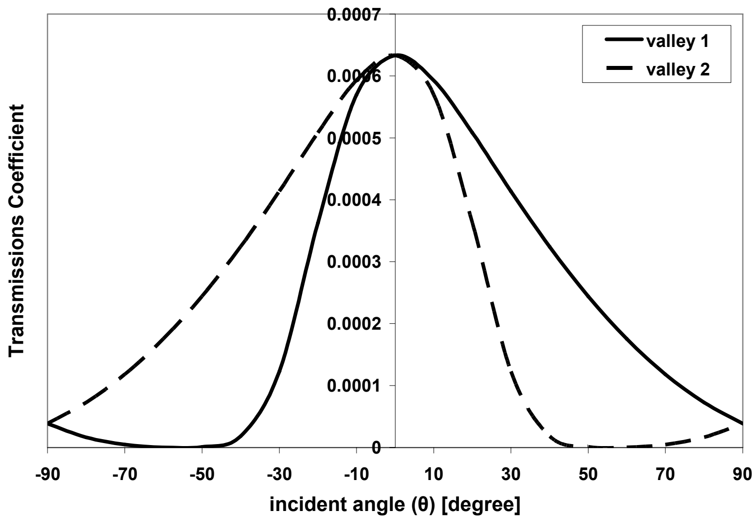

Figure 3 The transmission coefficient for the incident angle varying from -90^o to 90^o with incident energy of 75 meV and applied voltage of 50 mV.

The transmission coefficient as a function of incident angle for incident energy of 75 meV and applied voltage of 50 mV is shown in Fig. 3. The solid line is for electrons in the valley 1 and dashed line is for those in the valley 2. We can see that the transmission coefficient for electrons in the valley 1 and valley 2 occurs at normal incident. In addition, the transmission coefficient becomes the lowest for -65^o<θ<-45^o (the valley 1) and 45^o<θ<65^o (the valley 2). 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].

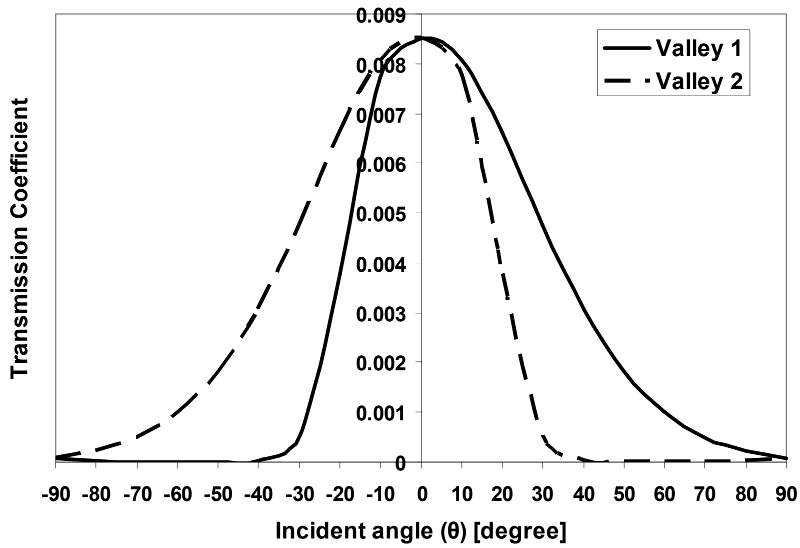

Figure 4 The transmission coefficient for the incident angle varying from -90^o to 90^o with incident energy of 150 meV and applied voltage of 50 mV.

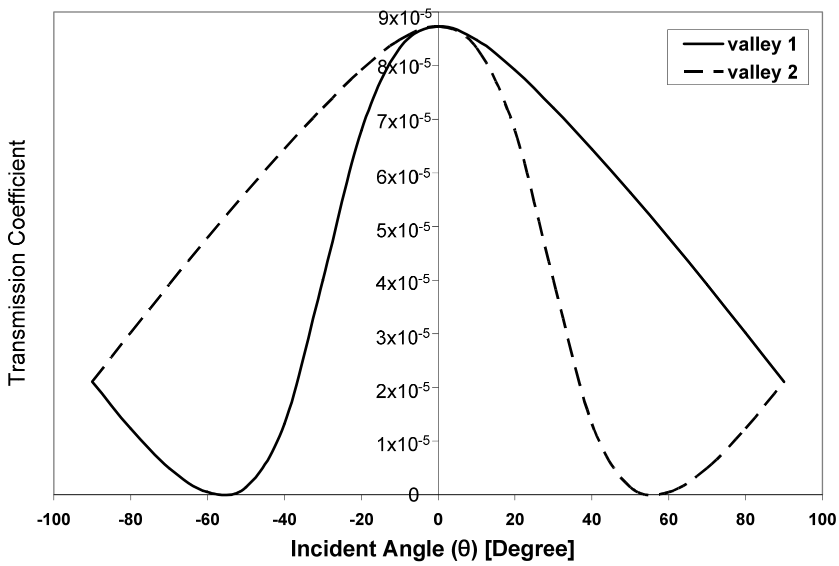

Figure 5 The transmission coefficient for the incident angle varying from -90^o to 90^o with incident energy of 25 meV and applied voltage of 100 mV.

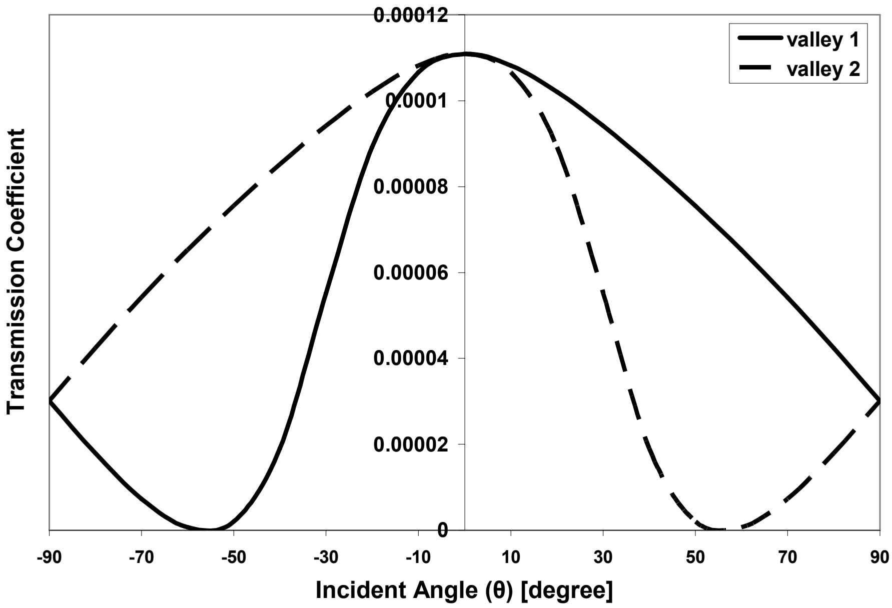

Figure 6 The transmission coefficient for the incident angle varying from -90^o to 90^o with incident energy of 25 meV and applied voltage of 150 mV.

In Fig. 4 the transmission coefficient for incident energy of 150 meV and applied voltage of 50 mV is presented. It is found that electron in the valley 1 and valley 2 have the highest transmission coefficient at about normal incidence. It is noted that the maximum value of the transmission coefficient for the incident energy of 75 meV is lower than that for the incident energy of 150 meV because the electrons have lower energy so that the probability of electrons to tunnel the barrier is also smaller. The incident angles having the lowest transmission coefficient becomes wider (-80^o<θ<-40^o and 40^o<θ<80^o) as the electron energy increases. It is probably due to the fact that if we increase the electron's incident energy then the energy in z direction is decreases. We also observe that for all valleys, the transmission coefficients are not symmetric with the incidence angle. If we decrease the incident energy, the electrons have lower energy to tunnel the potential barrier so that the probability of tunneling the barrier is smaller than that for the electrons with higher incident energy although bias voltage is increased as shown in Fig. 5. Transmission coefficient in Fig. 5 decrease two order of magnitude compare to transmission coefficient in Fig. 3. But for the same incident energy, the transmission coefficient will increase when the applied voltage to the barrier increased as shown in Fig. 6. In Fig 5 and 6, the maximum transmission coefficient is 9 x 10^{-5} and 11 x 10^{-5}, respectively. For the case in Figs. 5 and 6, the transmission coefficient is maximum at normal incident. We also see that, in all valleys, the transmission coefficient is not symmetric with the change of sign of incidence angle ($\theta \rightarrow -\theta$), which confirms the anisotropic of the materials [2].

4 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. 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 transmission coefficient will increase if the incident energy is increased. For the same incident energy, the highest value of the transmission coefficient occurs if the applied voltage to the barrier is high. The result shows that the transmission coefficient depends on the valley and it is not symmetric with the angle of incidence.

Acknowledgement

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

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