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An Improved Analytic Method Based on Airy Functions Approach to Calculate Electron Direct Transmittance in Anisotropic Heterostructure with Bias Voltage

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Abstract

An analytic expression of transmittance based on the Airy wavefunctions approach has been derived for an electron through an anisotropic heterostructure with an applied voltage to the barrier of the heterostructure. The Si(110)|$Si_{0.5}Ge_{0.5}$|Si(110) heterostructure was used to examine the analytic expression. In order to evaluate the Airy wavefunctions approach, the transfer matrix method, which is a method widely applied for various applications, was employed as a reference. It was found that the transmittance calculated by the Airy wavefunctions approach fits perfectly that obtained by the transfer matrix method. The exponential wavefunctions approach in obtaining the transmittance was also evaluated. The transmittance obtained by the exponential wavefunctions is always lower than the transfer matrix method-based transmittance. As the electron total energy or applied voltage increases, the difference between the exponential wavefunctions- and transfer matrix method-based transmittances increases. Thus, the Airy wavefunctions approach improves the exponential wavefunctions approach to calculate the electron direct transmittance.

Keywords*: Airy wavefunction, Anisotropic heterostructure, Direct tunneling, Exponential wavefunction, Transfer matrix method, Transmittance*

1. Introduction

Tunneling phenomenon through a potential barrier is still of interest in the study of quantum transport in high speed heterostructure devices. Paranjape[1)] derived transmission coefficient of an electron in an isotropic heterostructure without applying a bias voltage[1)]. Kim and Lee[2)] calculated transmission coefficient of an electron tunneling through an anisotropic heterostructure with zero bias voltage by solving the effective-mass equation including off-diagonal effective-mass tensor elements[2,3)]. Khairurrijal, *et al*. derived electron direct tunneling time through a trapezoidal barrier, which is due to a bias voltage, grown on isotropic materials by employing the Wigner phase time[4)]. Very recently, we have reported electron direct transmittance in an anisotropic heterostructure with applying a bias voltage by following the method in Ref. 4 in which the exponential wavefunctions (EWFs) are used[5,6)]. Unfortunately, when we applied the method to obtain the transmittance for the Fowler-Nordheim tunneling case, then we found that the transmittance is higher than one, which indicates the violation of the energy conservation law and implies that the electron direct transmittances previously calculated as reported in Refs. 5 and 6 are inaccurate. This is due to the use of approximate solutions of the Schrödinger equation with a linear potential profile. On the other hand, Khairurrijal, *et al*.[7)] calculated field emission current for electrons confined in an isotropic silicon subsurface quantum well by employing generalized Airy wavefunctions, which are exact solutions of the Schrödinger equation with an arbitrary potential profile[7)].

In this paper, we present a method in calculating the electron direct transmittance in an anisotropic heterostructure with a bias voltage based on the Airy wavefunctions (AWFs). An analytic expression of the direct transmittance is derived. As a reference to evaluate the present calculation method, we use the transfer matrix method (TMM) which is widely applied in various problems[8-14)]. The calculated results are discussed in details. It will be shown that the present method based on the AWFs improves the calculated direct transmittances as compared to those obtained by the EWFs-based method.

2. Theoretical Model

The Hamiltonian for general anisotropic materials is[2)]

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

where m_o is the mass of free electron, $\mathbf{p}$ is the momentum vector, $(1/m_o)\alpha$ is the inverse effective-mass tensor and $V(\mathbf{r})$ is the potential energy with the potential profile as given in Fig. 1 is expressed as

$$V(z) = \begin{cases} 0 & for \quad z \le 0 \\ \Phi - \dfrac{eV_b}{d} z & for \quad 0 < z < d \\ -eV_b & for \quad z \ge d. \end{cases} \tag{2}$$

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.

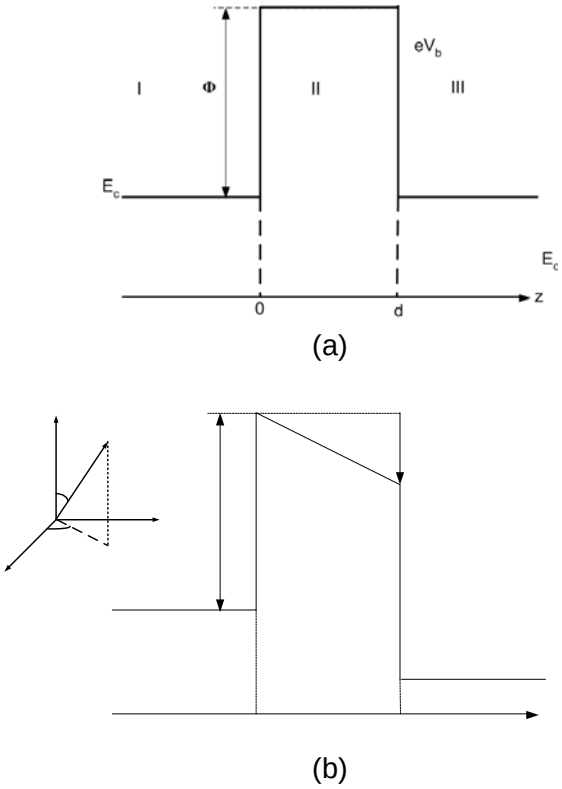

Figure 1. The potential profiles of a heterostructure (a) without a bias voltage and (b) with the application of a voltage to the barrier.

The effective mass of the electron and potential are position dependent only on the z direction. The wave function of the effective-mass equation with the Hamiltonian, as shown in Eq. (1), is given as [2]

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

and

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

is the wave number parallel to the interface.

By employing the separation variable to Eq. (1), it is 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 and the subscript l in $\alpha_{zz,l}$ denotes each region in Fig. 1. Here

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

is the electron energy at z direction, where

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

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.

2.1 The Airy Wavefunctions (AWFs) Approach

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

$$\Psi_1(z) = (Ae^{ik_1 z} + Be^{-ik_1 z})e^{-(i\gamma_1 z)}e^{-(ik_x x + ik_y y)},$$
$$\text{for } z \le 0, \tag{9}$$

$$\psi_2(z) = \left(C\mathrm{Ai}(\xi(z)) + D\mathrm{Bi}(\xi(z))\right)e^{-i\gamma 2z}e^{-i(k_x x + k_y y)},$$
$$\text{for } 0 < z < d, \tag{10}$$

$$\Psi_3(z) = Fe^{ik_3 z}e^{-(i\gamma_1 z)}e^{-(ik_x x + ik_y y)}. \quad \text{for } z \ge d. \tag{11}$$

The wave number k_1 and k_3 are expressed, respectively, as follows

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

and

$$k_3 = \left\{\frac{2m_o(E_z + eV_b)}{\hbar^2}\frac{1}{\alpha_{zz,1}}\right\}^{1/2}. \tag{13}$$

The argument $\xi(z)$ of the Airy functions Ai and Bi is

$$\xi(z) = \left(\frac{2m_0}{\hbar^2}eF\frac{1}{\alpha_{m,2}}\right)^{\frac{1}{3}} \left(-z + \frac{\Phi - E_z}{eF} - \frac{\hbar^2}{2m_0}\frac{1}{eF}\sum_{i,j\in(x,y)}(\beta_{ij,1} - \beta_{ij,2})k_i k_j\right) \tag{14}$$

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

$$\psi_1(z = 0^-) = \psi_2(z = 0^+), \tag{15a}$$

$$\frac{1}{m_o}\left[\alpha_{zx,l}\frac{d\psi_1}{dz} + \alpha_{zy,l}\frac{d\psi_1}{dz} + \alpha_{zz,l}\frac{d\psi_1}{dz}\right]_{z=0^-} = \frac{1}{m_o}\left[\alpha_{zx,2}\frac{d\psi_2}{dz} + \alpha_{zy,2}\frac{d\psi_2}{dz} + \alpha_{zz,2}\frac{d\psi_2}{dz}\right]_{z=0^+}, \tag{15b}$$

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

$$\frac{1}{m_o}\left[\alpha_{zx,2}\frac{d\psi_2}{dz} + \alpha_{zy,2}\frac{d\psi_2}{dz} + \alpha_{zz,2}\frac{d\psi_2}{dz}\right]_{z=d^-} = \frac{1}{m_o}\left[\alpha_{zx,1}\frac{d\psi_3}{dz} + \alpha_{zy,1}\frac{d\psi_3}{dz} + \alpha_{zz,1}\frac{d\psi_3}{dz}\right]_{z=d^+}, \tag{15d}$$

we will obtain the transmission amplitude T_a from Eqs. (9) - (11), which can be written as

$$T_a = \frac{F}{A}. \tag{16}$$

z k θ I Φ II y φ

Here,

$$\frac{F}{A}=\frac{2ik_1\alpha_{zz1}p_1}{\left(\frac{2m_o}{\hbar^2}\alpha_{zz2}^2eF\right)^{1/3}p_2+i(\alpha_{zz1}k_1p_3+\alpha_{zz1}k_3p_4)+\left(\frac{2m_o}{\hbar^2}\alpha_{zz2}^2eF\right)^{-1/3}k_1k_2\alpha_{zz1}p_5} \quad (17)$$

where

$$p_1=\mathrm{Ai}(\xi(d))\mathrm{Bi}'(\xi(d))-\mathrm{Bi}(\xi(d))\mathrm{Ai}'(\xi(d)) \quad (18)$$

$$p_2=\mathrm{Ai}'(\xi(d))\mathrm{Bi}'(\xi(0))-\mathrm{Bi}'(\xi(d))\mathrm{Ai}'(\xi(0)) \quad (19)$$

$$p_3=\mathrm{Ai}(\xi(0))\mathrm{Bi}'(\xi(d))-\mathrm{Bi}(\xi(0))\mathrm{Ai}'(\xi(d)) \quad (20)$$

$$p_4=\mathrm{Ai}(\xi(d))\mathrm{Bi}'(\xi(0))-\mathrm{Bi}(\xi(d))\mathrm{Ai}'(\xi(0)) \quad (21)$$

$$p_5=\mathrm{Ai}(\xi(d))\mathrm{Bi}(\xi(0))-\mathrm{Bi}(\xi(d))\mathrm{Ai}(\xi(0)). \quad (22)$$

2.2 The Transfer Matrix Method (TMM)

The TMM is based on dividing the domain of the solution into N segments as shown in Fig. 2 in which each segment of the potential energy is assumed to be constant.

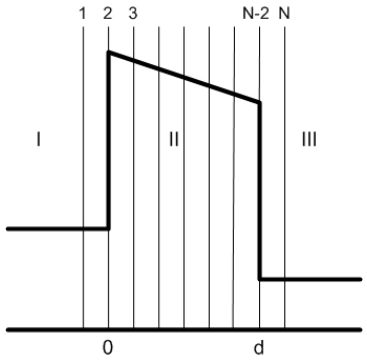

Fig. 2. The potential profile of a heterostructure is divided into N segments.

The time-independent electron wave function in each region is

$$\psi_1(z)=\left(A_1e^{ik_1z}+B_1e^{-ik_1z}\right)e^{-i\gamma_1z}e^{-i(k_xx+k_yy)} \quad (23)$$

$$\psi_j(z)=\left(A_je^{k_jz}+B_je^{-k_jz}\right)e^{-i\gamma 2z}e^{-i(k_xx+k_yy)} \quad (24)$$

$$\psi_N(z)=A_Ne^{ik_3z}e^{-i\gamma_1z}e^{-i(k_xx+k_yy)}, \quad (25)$$

where the wave number k_j is given in Eq. (26)

$$k_j^2=\frac{2m_0}{\hbar^2}\frac{1}{\alpha_{zz,2}}(\Phi-eFz)-\frac{\alpha_{zz,1}}{\alpha_{zz,2}}k_1^2 -\frac{1}{\alpha_{zz,2}}\sum_{i,j\in(x,y)}(\beta_{ij,1}-\beta_{ij,2})k_ik_j \quad (26)$$

By using the TMM we can easily get the following matrix

$$\begin{pmatrix}A_1\\B_1\end{pmatrix}=\begin{pmatrix}a_{11}&a_{12}\\a_{21}&a_{22}\end{pmatrix}\begin{pmatrix}A_N\\0\end{pmatrix}, \quad (27)$$

where a_{11}, a_{12}, a_{21}, and a_{22} are the matrix elements.

The transmission coefficient is given by

$$T_a=\frac{A_N}{A_1}=\frac{1}{a_{11}}. \quad (28)$$

The transmittance T is easily obtained by employing the following expressions

$$T=T_a^*T_a, \quad (29)$$

where T_a is given by Eqs. (16) or (18) for the AWFs approach or the TMM, respectively.

3. Calculated Results and Discussion

Following the model given in Fig.1, a strained $Si_{0.5}Ge_{0.5}$ potential barrier is on Si (110) so that the structure becomes $Si(110)|Si_{0.5}Ge_{0.5}|Si(110)$. The barrier width d and the band discontinuity Φ were taken as 5 nm and 216 meV, respectively[2]. There are four equivalent valleys in the conduction bands of Si (110) and strained $Si_{0.5}Ge_{0.5}$. Since the effective mass tensor elements of these four valleys are not the same, there are two groups of valleys in the Si (110) and $Si_{0.5}Ge_{0.5}$ as shown in Table 1 [2]. We calculated electron direct transmittances by applying the EWFs and AWFs approaches as well as the TMM. For the simplicity in the calculation we fixed φ to π/2.

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

The transmittance as a function of the incident angle for an electron with the total energy of 75 meV and applied voltage of 50 mV is shown in Fig. 3. We see that the transmittance obtained under the AWFs approach is the same as that calculated by the TMM but the EWF approach results in lower transmittance as compared to the TMM. The deviation of the transmittance calculated by the EWFs approach becomes significantly observed for small incident angles.

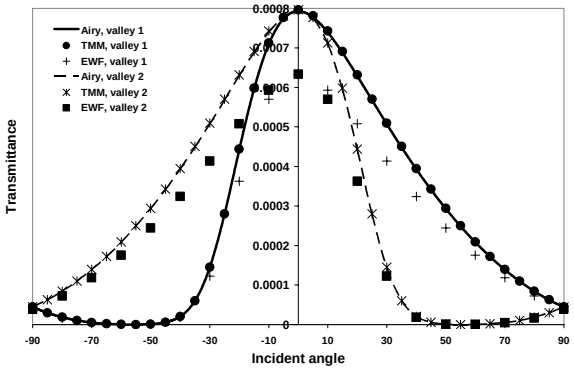

Figure 3. The transmittance for the incident angle varying from -90° to 90° with total energy of 75 meV and applied voltage of 50 mV.

Figure 4 gives the transmittance with the total energy of 150 meV and applied voltage of 50 mV. The maximum transmittances are still at the normal incidence and higher than those for the total energy 75 meV. Again, we see that the transmittance obtained under the AWFs approach replicates perfectly that calculated by the TMM. Significant difference in the transmittances occurs at small incident angles. As the applied voltage is increased for constant total energy, the difference in the transmittances becomes higher as clearly seen by comparing Figs. 3 and 4.

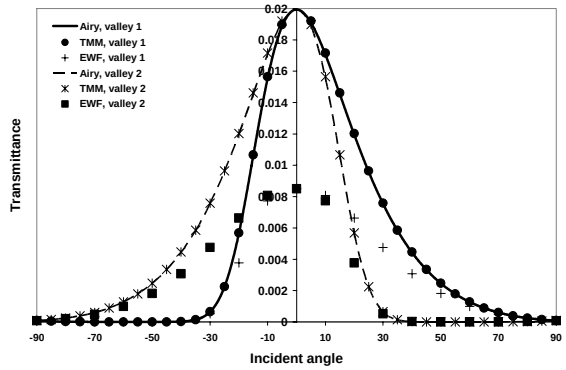

Figure 4. The transmittance for the incident angle varying from -90° to 90° with total energy of 150 meV and applied voltage of 50 mV.

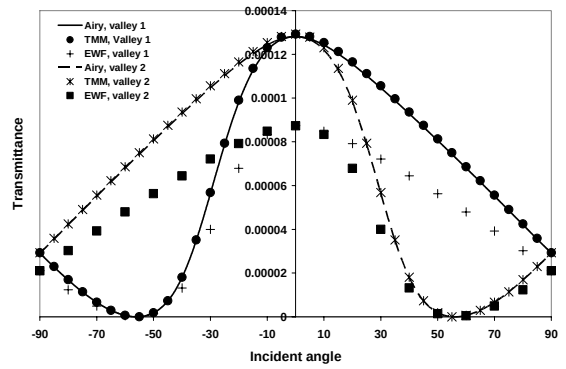

Figure 5 The transmittance for the incident angle varying from -90° to 90° with total energy of 25 meV and applied voltage of 100 mV.

Figures 5 and 6 depict the transmittances for the applied voltage of 100 mV and 150 mV, respectively. Again, we can see that the transmittances calculated by the AWFs and the TMM approaches fit very well. The discrepancy between the transmittances obtained by the EWFs and the AWFs approaches occurs at all incident angles. It can also be seen that the difference in the transmittances increases with increasing the applied voltage.

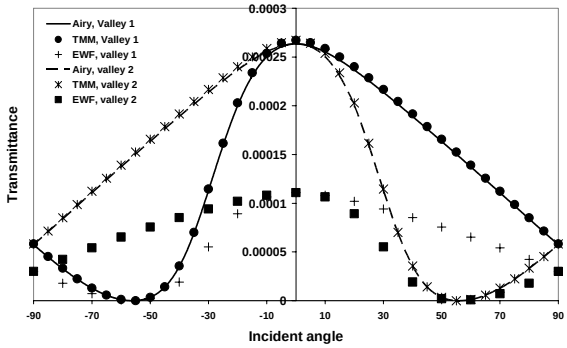

Figure 6. The transmittance for the incident angle varying from -90° to 90° with total energy of 25 meV with applied voltage of 150 mV.

Considering the valleys, we find from Figs. 3 to 6 that the transmittances for the valley 1 are the mirror of those for the valley 2. We also find that the transmittance is not symmetric with the change of sign of incident angle ($\theta \rightarrow -\theta$) for all valleys. This confirms the anisotropic properties of the materials[2].

Conclusion

We have derived an analytical expression of transmittance of electron through a nanometer-thick trapezoidal barrier grown on anisotropic materials based on the Airy wavefunctions (AWFs) approach. The calculation was applied to the Si(110)|$Si_{0.5}Ge_{0.5}$|Si(110) heterostructure. The calculated transmittance was compared to that obtained by the transfer matrix method (TMM), which is a method widely used for various applications. It was found that the AWFs-based transmittance reproduces perfectly the TMM-based one. The exponential wavefunctions (EWFs) approach in calculating the transmittance was also evaluated. The EWFs-based transmittance is always lower than that obtained by the TMM. The difference between the EWFs- and TMM-based transmittances increases with the increase of electron total energy or applied voltage. Therefore, the AWFs approach improves the EWFs approach in obtaining electron direct transmittance.

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