TUNNELING TIME AND TRANSMISSION COEFFICIENT OF AN ELECTRON TUNNELING THROUGH A NANOMETER-THICK SQUARE BARRIER IN AN ANISOTROPIC HETEROSTRUCTURE

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Abstract. Analytical expressions of transmission coefficient and tunneling time of electrons incident on a heterostructure grown on an anisotropic material are derived by solving the effective-mass equation including off-diagonal effective-mass tensor elements. It is 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 are applied to the Si(110)/$Si_{0.7}Ge_{0.3}$/Si(110) heterostructure, in which the SiGe barrier thickness is several nanometers. The calculated results shows that the transmission coefficient and the tunneling time are depend on the valley and it is not symmetric with the angle of incidence.
Key-words: Anisotropic material, heterostructure, nanometer-thick barrier, transmission coefficient, tunneling time.

1 Introduction

The tunneling phenomenon through a potential barrier has been discussed for last half century and also is of present day interest in the study of charge transport in a heterostructure. Paranjape has studied tunneling time and transmission coefficient of an electron in an isotropic heterostructure with different effective masses [1]. Kim and Lee have derived the electron tunneling time, post-tunneling position and transmission coefficient in a heterostructure barrier grown on anisotropic materials including off-diagonal effective-mass tensor elements [2]. In this paper, we report a theoretical study on the direct tunneling time and transmission coefficient of an electron in a heterostructure with nanometer-thick barrier grown on an anisotropic material with electron propagation direction making an arbitrary angle with respect to the interfaces of the heterostructure.

2 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

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

is the Hamiltonian, 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.

Figure 1 shows the potential profile in the normal direction (z direction) to the layer. The electron is incident from region I to potential barrier. The effective mass of the electron and potential are dependent only on the z direction. Φ is the potential barrier height due to band discontinuity of Si(110) and $Si_{0.7}Ge_{0.3}$ and d is the barrier width. The wave function of the effective-mass equation with the Hamiltonian of Eq. (1) is given as [2]:

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

where

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

is the wave number parallel to the interface. By substituting Eq (2) into Eq (1) it is found that $\varphi(z)$ satisfies the one dimensional Schrödinger-like equation:

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

where the subscript l in $\alpha_{zz,l}$ denotes each region in Fig. 1. Energy in the z direction can be then written as

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

where

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

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

and α_{ij} is the tensor elements associated with the inverse effective mass tensor.

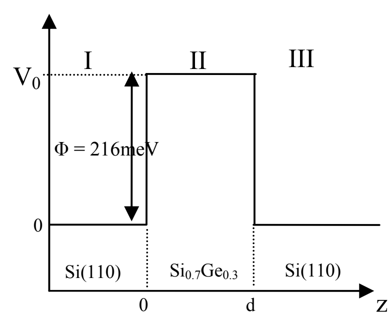

Fig 1. The model used in the numerical calculation

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

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

$$\Psi_2(z) = (Ce^{-\int_0^z k_2(z)dz} + De^{\int_0^z k_2(z)dz})e^{-(i\gamma_2 z)}e^{-(ik_x x + ik_y y)} \quad \text{for } 0 < z < d, \tag{10}$$

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

The incident wave $A\exp(ik_1 z)$ has the wave number k_1 expressed as

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

where E is smaller than the barrier height Φ. The wave numbers k_2 and k_3 are given as follows

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

$$k_3 = \left\{ \frac{2m_o E_z}{\hbar^2} \frac{1}{\alpha_{zz,I}} \right\}^{1/2}, \tag{14}$$

with the continuity conditions of the wavefunction at z = 0 and z = d given by [2] :

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

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

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

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

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

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

With these boundary conditions we obtain the transmission amplitude T_a as :

$$T_a = G\exp(i\phi), \tag{16}$$

where

$$G = \frac{2k_1 k_2}{(P^2 \sinh^2(u) + Q^2 \cosh^2(u))^{1/2}}, \tag{17}$$

is the amplitude of T_a,

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

is the phase of T_a,

$$P = \left(\frac{\alpha_{zz,I}}{\alpha_{zz,2}} k_1^2 - \frac{\alpha_{zz,2}}{\alpha_{zz,I}} k_2^2 \right), \tag{19}$$

$$Q = 2k_1 k_2, \tag{20}$$

$$u = k_2 d. \tag{21}$$

The transmission coefficient is easily obtained from

$$T = T_a^* T_a. \tag{22}$$

The direct tunneling time of an electron through the square barrier is [2]:

$$T_T = \frac{m_o}{\hbar k_3} \frac{1}{\alpha_{zz3}} \left(\frac{\partial \varphi(k_3)}{\partial k_3} + d \right), \tag{23}$$

Substituting Eq. (18) into Eq. (23), for energies lower than the potential barrier, we get

$$T_t = \frac{m_o}{\hbar k_3} \frac{1}{\alpha_{zzI}} \times \left\{ \frac{\left[k_1^2 k_2^2 \left(\frac{\alpha_{zz,1}}{\alpha_{zz,2}} + 1 \right) + k_1^4 \left(\frac{\alpha_{zz,1}}{\alpha_{zz,2}} \right)^2 + \frac{\alpha_{zz2}}{\alpha_{zz,1}} k_2^4 \right] \sinh(2k_2 d)}{k_2 [4k_1^2 k_2^2 \cosh^2(k_2 d) + P^2 \sinh^2(k_2 d)]} - \frac{2k_1^2 k_2 d \frac{\alpha_{zz,1}}{\alpha_{zz,2}} P}{k_2 [4k_1^2 k_2^2 \cosh^2(k_2 d) + P^2 \sinh^2(k_2 d)]} \right\}. \tag{24}$$

3 Calculated results and discussion

Referring to Fig. 1, a strained $Si_{0.7}Ge_{0.3}$ potential barrier (region II) is grown on Si (110) in region I or III. The width of the barrier is 50 Å and the band discontinuity is taken as 216 meV [2].

There are four equivalent valleys in the conduction band of Si (110). The effective mass tensor elements of these four valleys are not the same. There are two groups of valleys in Si (110) and $Si_{0.7}Ge_{0.3}$. The inverse effective masses used in our example are related to the tensor elements a_{ij} in Table 1 [3].

Table I. Tensor elements (a_{ij}) used in the numerical calculation.

Valley	Region I, III			Region II		
1	5.26	0	0	5.91	0	0
	0	3.14	2.12	0	3.86	2.45
	0	2.12	3.14	0	2.45	3.86
2	5.26	0	0	5.91	0	0
	0	3.14	-2.12	0	3.86	-2.45
	0	-2.12	3.14	0	-2.45	3.86

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 shown in Fig. 2, Eq. (7) becomes

$$
\begin{aligned}
E = {} & \frac{\hbar^2}{2m_o} \\
& \times \Big\{ \alpha_{xx1} k^2 \sin^2\theta \cos^2\varphi + \alpha_{yyx1} k^2 \sin^2\theta \sin^2\varphi + \alpha_{zz1} k^2 \cos^2\theta \\
& 2\Big(\alpha_{xy1} k^2 \sin^2\theta \cos\varphi \sin\varphi + \alpha_{yz1} k^2 \sin^2\theta \cos\theta \sin\varphi \\
& + \alpha_{zx1} k^2 \sin^2\theta \cos\theta \cos\varphi \Big)\Big\}
\end{aligned}
\tag{25}
$$

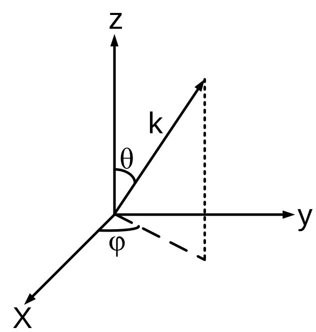

Fig.2. The coordinates used in the analysis.

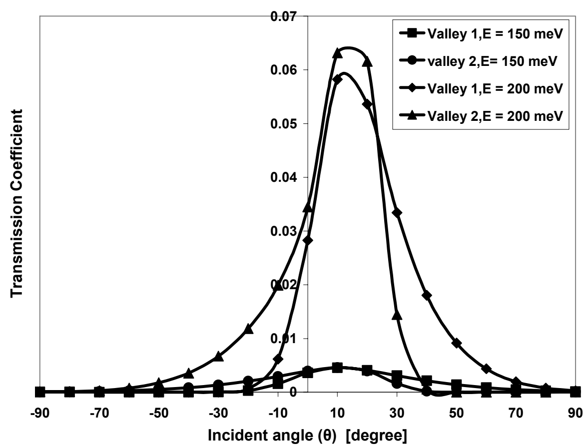

Fig 3. The transmission coefficients for the angle of incident varying from -90° to 90° with incident energies of 150 meV and 200 meV

We calculate the transmission coefficient for the incident angle of **k** (the wave vector of incident electron) varying from -90° to 90° with incident energies of 150 meV and 200 meV and the results are plotted in Fig. 3. Although the incidence angles are θ and φ, but we fix φ to π/2 for simplicity. It can be seen that the transmission coefficient for the incident energy of 200 meV is higher than that for the incident energy of 150 meV. This is because electrons have energy high enough to tunnel the barrier. For all valleys, the transmission coefficient is maximum not for normal incident but at the incident angle of about 10°. This is due to fact that motions in the x and y directions are not independent of that in the z direction, but they are mutually coupled by the off-diagonal effective-mass tensor elements [4].

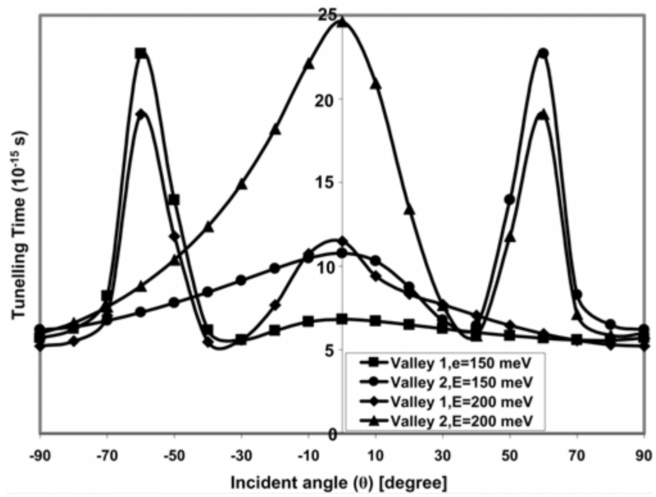

Fig 4. The tunneling time for the angle of incident varying from -90° to 90° with incident energies is 150 meV

The tunneling time versus incident angle is given in Fig.4. We see that the tunneling time depends on the valley where the electron belongs and the incident angle of **k**. It is noteworthy that, in all valleys, the tunneling time is not symmetric with the change of sign of the incidence angle (θ→-θ), which confirms the anisotropy of the material. For the valley 1, the tunneling time has a primary peak at the angle θ of -60° for the incident energy of 150 meV while the secondary peak occurs at the angle of about 0° for the incident angle of 200 meV. For the valley 2, electron with the incident energy of 200 meV have the longest tunneling time at θ = 0°. If the incident angle increases, the next peak of the tunneling time takes place at θ = 60° for the energy of 150 meV.

4 Conclusion

We have derived analytical expressions of the direct tunneling time and transmission coefficient of an electron in a nanometer-thick square barrier grown on anisotropic materials under non-normal incidence. We included the effect of different effective masses at heterojunction interfaces. 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 calculation is done with a $Si_{0.7}Ge_{0.3}$ potential barrier grown on Si (110). The calculation shows that the transmission coefficient and the tunneling time depend on the valley and it is not symmetric with the angle of incidence.

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