Spin Dependent Tunneling through a Nanometer-thick Square Barrier Based on Zinc-blende Structure Material

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Abstract

*Spin dependent tunneling through a nanometer thick square barrier based on zinc- blende structure material has a great deal of attention due to its potential application in spintronics devices. An analytic expression of the transmittance T of an electron with spin polarization has been derived by adding the Dresselhauss term to the commonly used Hamiltonian and solving the Schrödinger equation. Solutions of the Schrödinger equation give two states referred as the "up" or "+" and "down or "-" spin states. It was found that the "up" and the "down" state transmittances are asymmetric to the axis at the normal incidence (*θ*=0^o). Moreover, at the normal incidence the transmittances are equal because the parallel wave vectors are zero and not the highest. In addition, it was also found the relation* $T_+(\theta) = T_-(-\theta)$ due to the anisotropic *properties of heterostructure materials.*

Keywords: Dresselhauss term, Spin dependent tunneling, Spin polarization, Transmission coefficient, Transmittance, Zincblende material

1. Introduction

In recent years, many theoretical and experiment works on spintronics have been conducted because of the scientific interest in spin-dependent transport of electrons as well as technological applications^{1,2)}. Many authors have revealed that the spin-dependent transport in semiconductor heterostructures can be achieved by using ferromagnetic semiconductor materials $3-6$) following the invention of diluted magnetic semiconductor (DMS) by Ohno⁷. On the other hand, Voskoboynikov, *et. al.*⁸) suggested that a spin filter could be obtained from nonmagnetic semiconductor material due to the Rashba spin-orbit coupling^{8,9)}. Flatte, *et. al.*^{10,11}) proposed a spin transistor by taking advantage of the unique characteristics of bulk inversion asymmetry in (110) oriented nonmagnetic semiconductor heterostructures. Perel' *et. al.*¹²⁾ found that electron tunneling through a zinc-blende semiconductor depends on spin polarization. Moreover, the Dresselhaus effect arising in the zincblende semiconductor produces interface current enhancement in thin barrier case as reported by Wang *et. al*13).

In this paper, we present the study on electron tunneling through a nanometer-thick zinc-blende semiconductor square barrier with spin consideration. By incorporating the Dresselhaus term to the Hamiltonian and solving the Schrödinger equation, we obtained an analytical expression of electron transmittance, which depends on spin orientation. We calculated the electron transmittance and polarization as functions of energy in the normal direction and incident angle. Then, the calculated results are discussed thoroughly.

2. Theoretical Model

The potential profile of a semiconductor heterostructure is shown in Fig. 1. The heterostructure is composed of three regions, in which the material in region \mathbf{I} is the same as that in region III and the zinc-blende semiconductor in region II acts as a potential barrier. The barrier width and height are *L* and *V*0, respectively. An electron comes from the region I to the potential barrier with the initial wave propagation vector given by Eq. (1) .

$$
\vec{k} = k_{\rho} \hat{\rho} + k_{z} \hat{z}, \tag{1}
$$

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$$

where $\hat{\rho}$ and \hat{z} are the unit vectors in parallel and normal directions to the interfaces between two regions, respectively. The incident angle θ is expressed as $\theta = \arctan(k_{\rho} / k_z)$, where k_{ρ} and k_z are the momentum in parallel and normal directions, respectively.

The electron behavior in the heterostructure is described by Schrödinger equation

$$
H\Psi = E\Psi , \qquad (2)
$$

where E is the electron total energy and Ψ is the electron wave function. The Hamiltonian H comprises H_0 , which is common for the heterostructure without consideration of spin¹⁴⁾, and H_D is the Dresselhaus term for taking into account the spin.

Figure 1. Potential profile of a heterostructure and incident electron wave vector

The Dresselhaus term H_D is given by^{12,15)}

$$
H_D = \gamma (\sigma_x k_x - \sigma_y k_y) \frac{\partial^2}{\partial z^2} , \qquad (3)
$$

where γ is the Dresselhaus constant and σ_i with $i = x, y$, and *z* are the Pauli matrices. The wave number k_x and k_y are related to the wave number k_{ρ} in the xy plane so that $\vec{k}_\rho = k_x \hat{x} + k_y \hat{y}$ with \hat{x} and \hat{y} are the unit vectors in the xy plane.

It can be found that the Dresselhauss term in Eq. (3) has the "eigen value problem" form with the eigen states-like

$$
\chi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mp e^{-i\varphi} \end{pmatrix}, \tag{4.a}
$$

and the eigen values-like

$$
\chi_{\pm} = \mp \gamma k_{\rho} \frac{\partial^2}{\partial z^2} \ . \tag{4.b}
$$

Here, φ is the polar angle of the wave vector in *xy* plane \vec{k}_ρ , so that

$$
\vec{k}_{\rho} = k_{\rho} \cos \varphi \hat{\mathbf{x}} + k_{\rho} \sin \varphi \hat{\mathbf{y}},
$$
 (5)

The subscripts "+" and "-" Eqs. $(4.a)-(4.b)$ refer to the electron spin states, which are often called "up" and "down", respectively.

The electron wave function and total energy in Eq. (2) can be written, respectively, as

$$
\Psi_{\pm}(\vec{r}) = \chi_{\pm} \phi_{\pm}(z) \zeta(\rho), \qquad (6)
$$

$$
E_{\pm} = E_{gr} + E_{z\pm} \tag{7}
$$

By employing the variable separation technique, it is obtained two differential equations expressed in Eqs. (8.a) and (8.b)

$$
-\frac{\hbar^2}{2m^*}\frac{d^2\zeta}{d\rho^2} = E_{\rho}\zeta , \qquad (8. a)
$$

$$
-\frac{\hbar^2}{2m_{\pm}^*}\frac{d^2\phi_{\pm}}{dz^2} + V(z)\phi_{\pm} = E_{zz}\phi_{\pm},
$$
 (8.b)

where

$$
m_{\pm}^{*} = m^{*} \left(1 \pm 2 \frac{m^{*} k_{\rho}}{\hbar^{2}} \right)^{-1}.
$$
 (9)

Solutions of the differential equation in Eq. (8.a) are easily obtained as given in Eqs. (10.a) and (10.b).
 $\zeta(\rho) = A \exp(i\vec{k}_o \cdot \vec{\rho})$, (10.a)

$$
\zeta(\rho) = A \exp(i\vec{k}_{\rho}.\vec{\rho}) ,
$$
\n
$$
E_{\rho} = \frac{\hbar^2 k_{\rho}^2}{2m^*} ,
$$
\n(10.b)

where the position in the xy plane is $\vec{\rho} = x\hat{x} + y\hat{y}$. Equation (8.b) gives solutions as written in Eqs. (11.a) and (11.b).

$$
\phi_{\pm} = \begin{cases}\n\exp(ik_{z1\pm}) + r_{\pm} \exp(-ik_{z1\pm}z), & \text{for } z < 0 \\
A_{\pm} \exp(k_{z2\pm}z) + B_{\pm} \exp(-k_{z2\pm}z), & \text{for } 0 < z < L \\
t_{\pm} \exp(ik_{z1\pm}z), & \text{for } z > L\n\end{cases}
$$
\n(11.a)

$$
E_{z\pm} = \frac{\hbar^2 k_{z\pm}^2}{2m_{1\pm}^*} \tag{11.b}
$$

where

$$
k_{z1\pm} = \left\{ \frac{2m_1^*}{\hbar^2} \left(E_{\pm} - \frac{\hbar^2 k_\rho^2}{2m_1^*} \right) \right\}^{1/2} \left(1 \pm \frac{2\gamma m_1^* k_\rho}{\hbar^2} \right)^{-1/2}, (12. a)
$$

$$
k_{z2\pm} \equiv \left\{ \frac{2m_2^*}{\hbar^2} \left(V_0 + \frac{\hbar^2 k_\rho^2}{2m_2^*} - E_\pm \right) \right\}^{1/2} \left(1 \pm \frac{2m_2^* k_\rho}{\hbar^2} \right)^{-1/2}, (12.b)
$$

$$
m_{1\pm}^* = m_1^* \left(1 \pm \frac{2\gamma m_1^* k_\rho}{\hbar^2} \right)^{-1}, \tag{13.3}
$$

$$
m_{2\pm}^* = m_2^* \left(1 \pm \frac{2\gamma m_2^* k_\rho}{\hbar^2} \right)^{-1},
$$
 (13.b)

and the subscript 1 and 2 represent the region 1 and 2, respectively.

Since the boundary conditions of our problem requires that ϕ_{\pm} and $m^{-1}(d\phi_{\pm}/dz)$ are continuous at the interfaces¹⁶, the transmission coefficient can be derived to be

$$
t_{\pm} = 2k_{z1\pm}k_{z2\pm} \exp(-ik_{z1\pm}L) \times \frac{\left\{2k_{z1\pm}k_{z2\pm}\cosh(k_{z2\pm}L) + i\left(\frac{m_{2\pm}^{*}}{m_{1\pm}^{*}}k_{z1\pm}^{2}-\frac{m_{1\pm}^{*}}{m_{2\pm}^{*}}k_{z2\pm}^{2}\right)\sinh(k_{z2\pm}L)\right\}}{\left\{2k_{z1\pm}k_{z2\pm}\cosh(k_{z2\pm}L)\right\}^{2} + \left\{\left(\frac{m_{2\pm}^{*}}{m_{1\pm}^{*}}k_{z1\pm}^{2}-\frac{m_{1\pm}^{*}}{m_{2\pm}^{*}}k_{z2\pm}^{2}\right)\sinh(k_{z2\pm}L)\right\}^{2}}.
$$
(14)

It can be seen that the transmission coefficient in Eq. (14), which is obtained by taking into account the spin is similar to that without the spin as derived by Khairurrijal *et. al.* in Ref 14. The differences are only in the wave number k_z and the effective mass m^* .

Therefore, the transmittance T_{\pm} for each state is easily calculated by using Eq. (15).

$$
T_{\pm} = t_{\pm}^* t_{\pm} \tag{15}
$$

where t_{\pm}^{*} refers to the complex conjugate of t_{\pm} .

For the incident electron that makes an arbitrary angle to the interface with total energy *E*, the wave number can be calculated by using

$$
k = \sqrt{\frac{2m^*E}{\hbar^2}} \tag{16.3}
$$

$$
k_{\rho} = k \sin \theta , \qquad (16.5)
$$

$$
k_z = k \cos \theta \,. \tag{16.c}
$$

Energy in the normal direction E_z can be obtained from Eq. (16.c), and then the transmittance is calculated by using Eq. (15).

It is suitable to introduce the polarization of spin *P* which is defined as

$$
P = \frac{T_+ - T_-}{T_+ + T_-} \times 100\% \,. \tag{15}
$$

It means that if the transmittance of the "+" state is dominant as compared to that of the "-" state then *P* becomes positive. When the transmittance of the "-" state become influentially then *P* is negative.

3. Calculated Results and Discussion

We used Metal-GaSb-Metal heterostructures in our calculation. The barrier height V_0 of GaSb is 0.2 eV¹³⁾. The Dresselhaus constant (*γ*) of metal and GaSb zincblende semiconductor are 0 and 187 eV \AA^{-3} , respectively^{12,13}. Since γ in the region I is the same as that in the region III, the wave vectors are also the same.

Figure 2. Transmittance for incident wave number k_o = $10⁹m⁻¹$ and barrier width $L = 5$ nm

Figure 2 and 3 depict the electron transmittance *T* for "up" $(+)$ and "down" $(-)$ spin states as a function of the electron energy in the normal direction E_z with the wave number k_{ρ} of 10⁹/m and the barrier width *L* of 5 and 10 nm, respectively. It is shown that the transmittance *T* increases with energy in the normal direction E_z for E_z lower than the barrier height V_0 of 0.2 eV. Further increase of E_z results in oscillation of T . The oscillatory behavior of *T* is the same as that for electron tunneling without spin consideration 17 . However, the inclusion of spin splits the resonant energy E_r , in which $T(E_r)$ is equal to 1. For the barrier width *L* of 5 nm, the first resonant energies overlap near 0.21 eV and the second ones are 0.49 and 0.64 eV for the "down" and "up" spin states, respectively, as shown in Fig. 2. For *L* of 10 nm as given in Fig. 3, we find that the first resonant energies are identical to those for *L* of 5 nm, the second resonant energies are 0.28 and 0.31 eV for "down" and "up" spin states, respectively, and the third ones are the same as the second resonant energies for *L* of 5 nm.

Figure 3. Transmittance for incident wave number k_{ρ} = $10⁹$ m⁻¹ and barrier width $L = 10$ nm

Figure 4. Polarization for incident wave number *k*^ρ 10^9 m⁻¹, and barrier width $L = 5$ and 10 nm.

Figure 4 plots the polarization *P* with conditions that are the same as those for Figs. 2 and 3. It is found that the polarization has positive values and it decreases

with the electron energy in the normal direction E_z for E_z lower than barrier height V_0 . It means that the "up" state is more dominant than the "down" state. For *Ez* higher than V_0 , the polarization oscillates between the positive and negative values. When *P* is positive, the "up" state is dominant as compared to the "down" state. As the "down" state becomes dominantly, *P* becomes negatives. It is interesting to note from Figs. 2 and 4 that the zero polarizations, which occur when T_+ is equal to T_- , appear at *Ez* of 0.21 eV (*T* = 1) and 0.56 eV (*T* = 0.75) for *L* of 5 nm. For *L* of 10 nm, the zero polarizations also appear at E_z of 0.29 eV ($T = 0.88$), 0.38 eV ($T = 0.36$), and 0.74 eV ($T = 0.35$) in addition to those observed for *L* of 5 nm.

Figure 5. Transmittance as a function of incident angle with incident total energy *E* of 0.1 eV and barrier width *L* of 5 and 10 nm.

Figures 5 and 6 show the electron transmittance for incident angle θ varying from -90 $^{\circ}$ to 90 $^{\circ}$, with the barrier width *L* of 5 and 10 nm and incident total energy *E* of 0.1, and 0.2 eV, respectively. It is seen that the transmittance coefficient for each state does not overlap and is not symmetric because of the bulk inversion asymmetry 10^{-11}) of the zinc-blende structure. The highest transmittance for the incident total energy *E* of 0.1 eV is not in the normal direction, but it occurs at about $\pm 2^{\circ}$. The transmittance decreases as the incident angle increases. For the incident angle larger than $\pm 45^\circ$ the transmittance is very low. For *E* of 0.2 eV we find that the highest transmittance is at the incident angle of 0° . The transmittance becomes infinitely low for the incident angle larger than $\pm 30^{\circ}$. Furthermore, the increase in the incident total energy *E* from 0.1 to 0.2 eV results in significant increase in the highest transmittance. It is seen that the transmittance of the "down" state electron is greater than that of the "up" state electron for negative incident angles while for positive incident angles vice versa. At the normal incidence $(\theta = 0^{\degree})$ the transmittances for both states are equal because their parallel wave vectors become zero and thus their effective masses expressed in Eq. (13.a) or (13.b) are the same. Although the transmittance is asymmetric, it was found the relation T₊(θ)= T₋($-\theta$). This result is similar to that obtained by Kim and Lee due to the anisotropic properties of heterostructure materials.¹⁸⁾ We also suggest to explore

the result using the group theory, which is beyond the scope of the present discussion.

Figure 6. Transmittance as a function of incident angle with incident total energy *E* of 0.2 eV and barrier width *L* 5 and 10 nm.

Figure 7 illustrate the polarization *P* of spin of electron tunneling with variation of incident angle *θ* for the incident energy *E* of 0.1 and 0.2 eV and the barrier width *L* of 5 and 10 nm. It is shown that the polarization increases with increasing the incident angle. For the incident angle near the parallel direction $(\pm 90^\circ)$, the polarization is much higher than that for the incident angle near the normal direction (0°) . Therefore, the polarization is easier to occur if the incident angle nears the parallel direction. Although the polarization is high at θ near $\pm 90^\circ$, the transmittance is almost zero as shown in Figs. 5 and 6.

Figure 7. Electron spin polarization as a function of incident angle with incident energies of 0.1 and 0.2 eV.

4. Conclusion

We have derived an analytical expression of the transmittance of electron with spin tunneling through a nonmagnetic semiconductor square barrier by adding the Dresselhauss term to the commonly used Hamiltonian to consider the spin effect in a semiconductor heterostructure. Solutions of the Schrödinger equation give two states, which are referred as the "up" and "down" spin states. The transmittance was calculated for the heterostructure with the barrier made from the zincblende structure material. It was shown that either the

"up" or the "down" state transmittance is asymmetric to the axis at the normal incidence $(\theta = 0^{\circ})$. Although both transmittances are the same at the normal incidence because the parallel wave vectors are zero, the highest transmittances are not at this incident angle. In addition, it was found the relation $T_+(\theta) = T_-(-\theta)$ due to the anisotropic properties of heterostructure materials.

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