Comparison of electron transmittances and tunneling currents in an anisotropic $TiN_x/HfO_2/SiO_2$/p-Si(100) metal–oxide–semiconductor (MOS) capacitor calculated using exponential- and Airy-wavefunction approaches and a transfer matrix method

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Abstract: Analytical expressions of electron transmittance and tunneling current in an anisotropic $TiN_x/HfO_2/SiO_2$/p-Si(100) metal–oxide–semiconductor (MOS) capacitor were derived by considering the coupling of transverse and longitudinal energies of an electron. Exponential and Airy wavefunctions were utilized to obtain the electron transmittance and the electron tunneling current. A transfer matrix method, as a numerical approach, was used as a benchmark to assess the analytical approaches. It was found that there is a similarity in the transmittances calculated among exponential- and Airy-wavefunction approaches and the TMM at low electron energies. However, for high energies, only the transmittance calculated by using the Airy-wavefunction approach is the same as that evaluated by the TMM. It was also found that only the tunneling currents calculated by using the Airy-wavefunction approach are the same as those obtained under the TMM for all range of oxide voltages. Therefore, a better analytical description for the tunneling phenomenon in the MOS capacitor is given by the Airy-wavefunction approach. Moreover, the tunneling current density decreases as the titanium concentration of the TiN_x metal gate increases because the electron effective mass of TiN_x decreases with increasing nitrogen concentration. In addition, the mass anisotropy cannot be neglected because the tunneling currents obtained under the isotropic and anisotropic masses are very different.

Key words: Airy wavefunction; anisotropic MOS; exponential wavefunction; transfer matrix method; transmittance; tunneling current

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1. Introduction

For half a century, numerous theoretical and experimental investigations have been carried out to study electron tunneling processes in heterostructures[1−3]. A metal–oxide–semiconductor (MOS) capacitor, as one type of heterostructure, is aggressively scaled-down to nanoscale dimensions in order to improve its performance[4, 5]. However, the tunneling current increases and power dissipation becomes significantly high as the SiO_2 gate-dielectric thickness decreases[6]. Recently, a stack of SiO_2 and a high dielectric constant (high-k) oxide layer has been applied as the oxide layer in the MOS capacitor so that a high power-dissipation due to an enormous tunneling current can be reduced[7, 8].

Hafnium dioxide (HfO_2) as one of the high-k materials is a promising material in high-k integration in CMOS technology because it has good thermal stabilities and favorable energy band alignments to Si (100)[9]. On the other hand, the introduction of high-k materials is complemented by the surrogate of poly-Si gate electrodes by fresh gate electrode materials with an adaptable work function, such as metal nitrides[10]. By using metal nitrides as gate electrodes, the formation of a depletion layer in the poly-Si gate can be restrained in which trapped charge scattering effects are reduced[11]. Titanium nitride (TiN_x) with a high melting point, a high thermal conductivity, extreme hardness and good corrosion is the prospect material to be applied in the MOS technology as a metal gate[12]. In addition, the properties of TiN_x films actually depend considerably on their composition and vacancy density[13, 14].

The behavior of an electron in the MOS capacitor is described by the Schrödinger equation and it can be solved analytically or numerically. The exponential- and Airy-wavefunction approaches, which are two analytical approaches, have been used to compute electron direct transmittance and tunneling time and current in heterostructures under an isotropic mass, and without considering a coupling between transverse and longitudinal motions[15−22], and it has been found that the results of the Airy-wavefunction approach differ from those obtained from the exponential-wavefunction approach[23, 24]. Additionally, taking into account an isotropic mass and without including a transverse-longitudinal kinetic energy coupling, the transmittance and tunneling current in heterostructures have been calculated under a transfer matrix method (TMM), which is often used to solve the Schrödinger equation numerically[25−28].

On the other hand, it is well known that silicon used as a substrate of the MOS capacitor has an anisotropic mass. In addition, it has been shown that the coupling of transverse and longitudinal energies is important in heterostructures including MOS capacitors[29]. However, analytical methods for obtaining the transmittance and tunneling current in the MOS

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capacitor using the exponential- and Airy-wavefunction approaches under an anisotropic mass and taking into account the transverse-longitudinal kinetic energy coupling have not been performed.

In this paper, we report electron transmittance and tunneling current in a $TiN_x/HfO_2/SiO_2$/p-Si(100) MOS capacitor calculated analytically under the exponential- and Airy-wavefunction approaches by including the transverse-longitudinal kinetic energy coupling and anisotropic masses. The coupling of transverse and longitudinal kinetic energies is represented by the electron phase velocity in the TiN_x gate. The results are compared to those obtained under the TMM to find the best analytical approach in describing the tunneling process. In addition, the influence of the Ti composition of the TiN_x metal gate to the tunneling current is also presented.

2. Theoretical model

A schematic energy diagram of a $TiN_x/HfO_2/SiO_2$/p-Si(100) MOS capacitor in a flatband condition is depicted in Fig. 1(a). Here, φ_m is the metal work function, φ_{Si} is the work function of Si, χ is the electron affinity of Si, E_c and E_v are the conduction and valence bands of Si, respectively, $E_{F,Si}$ is the Fermi level of Si, and $E_{g,a}$, $E_{g,b}$ and $E_{g,Si}$ are the band gaps of HfO_2, SiO_2, and Si, respectively. Under a negative bias voltage applied to the TiN_x metal gate, electrons coming from the metal gate pass through the potential barrier and then arrive at the p-type silicon substrate. The potential profile of the conduction band energy is therefore given in Fig. 1(b) in which the conduction band differences between HfO_2 and Si, SiO_2 and Si, and TiN_x and Si are Φ_a, Φ_b, and Δ, respectively, and d_1 and $d_2 - d_1$ are the thicknesses of HfO_2 and SiO_2, respectively.

The potential profile in Fig. 1(b) is mathematically expressed as

$$V(z) = \begin{cases} 0, \quad z < 0, \\ (\Phi_a + \Delta) - \kappa_b p z, \quad 0 \leqslant z < d_1, \\ (\Phi_b + \Delta) + p d_1(\kappa_a - \kappa_b) - \kappa_a p z, \quad d_1 \leqslant z < d_2, \\ -(eV_{ox} - \Delta), \quad z \geqslant d_2, \end{cases} \tag{1}$$

where $p = \frac{eV_{ox}}{\kappa_a(d_2 - d_1) + \kappa_b d_1}$, e is the electronic charge, V_{ox} is the oxide voltage which is the voltage across the barrier, and κ_a and κ_b are the dielectric constants of HfO_2 and SiO_2, respectively.

Considering that the potential energy $V(z)$ is only dependent on the z-direction, an electron in anisotropic materials under the parabolic-band effective mass approximation is described as[30]

$$\left(\frac{1}{2}\boldsymbol{p}^T \frac{\alpha(\boldsymbol{r})}{m_0}\boldsymbol{p} + V(z)\right)\Theta(\boldsymbol{r}) = E\Theta(\boldsymbol{r}), \tag{2}$$

where $\boldsymbol{p}$ is the momentum vector, $\alpha(\boldsymbol{r})/m_0$ is the inverse effective-mass tensor, and E and $\Theta(\boldsymbol{r})$ are the electron total energy and wavefunction, respectively.

Since the total energy E is composed of the longitudinal (the z-direction) and the transverse (the x–y plane) energies and is written as $E = E_z + E_{xy}$, the wavefunction in the z-direction $\Psi(z)$ satisfies the one-dimensional Schrödinger-like equation as follows,

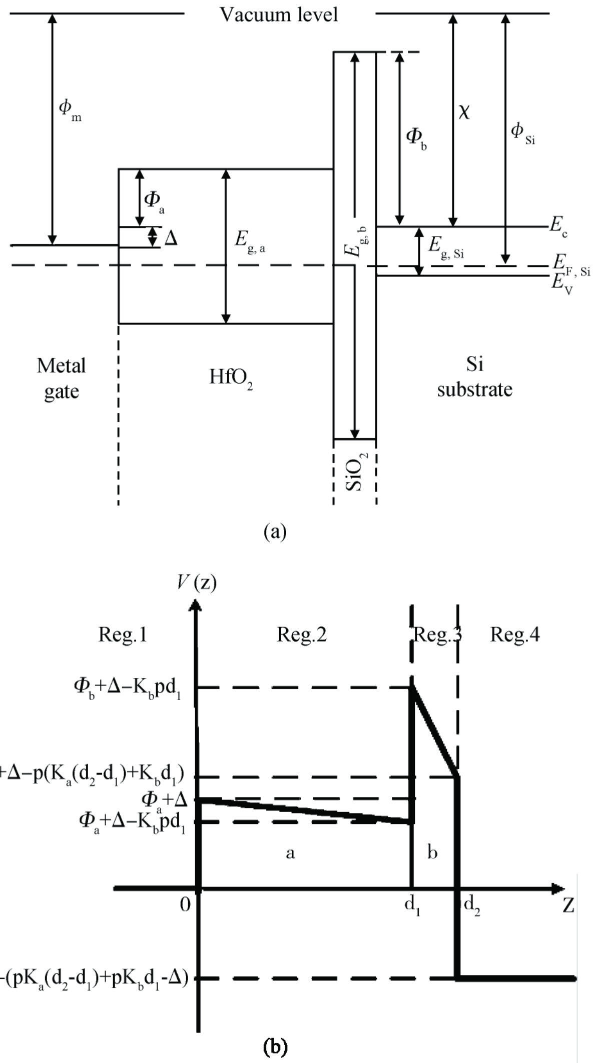

Fig. 1. (a) Energy band diagram of a $TiN_x/HfO_2/SiO_2$/p-Si MOS capacitor in a flatband condition. (b) Potential profile in the z-direction under a negative bias voltage applied to the TiN_x gate.

$$-\frac{\hbar^2}{2m_0}\alpha_{zz}\frac{d^2\Psi(z)}{dz^2} + V(z)\Psi(z) = E_z\Psi(z), \tag{3}$$

where $\hbar$ is the reduced Planck constant and $E_z = E - \sum_{i,j\in\{x,y\}} \frac{\hbar^2}{2m_0}\beta_{ij}k_i k_j$. Here, $\beta_{ij} = \alpha_{ij} - (\alpha_{iz}\alpha_{zj}/\alpha_{zz})$, α_{ij} is the tensor element of $\alpha(\boldsymbol{r})$, k_i is the wavenumber in the i-direction, and $i,\ j \epsilon \{x, y\}$.

Noting that the total energy is kept constant, the longitudinal energy in region $n \ \epsilon \ \{2, 3, 4\}$ with respect to that in region 1 is

$$E_{z,n} = E_{z,1} + \frac{\hbar^2}{2m_0}\sum_{i,j\in\{x,y\}}(\beta_{ij,1} - \beta_{ij,n})k_i k_j. \tag{4}$$

By substituting Eq. (4) into Eq. (3), it is found that

$$-\frac{\hbar^2}{2m_0}\alpha_{zz,n}\frac{d^2\Psi(z)}{dz^2} + V_{eff}(z)\Psi(z) = E_{z,1}\Psi(z), \tag{5}$$

where $V_{eff}(z)$ is the effective potential energy that is given by

$$V_{\text{eff}}(z) = V(z) - \sum_{i,j\in\{x,y\}} \frac{\hbar^2 k_i k_j}{2m_0}\beta_{ij,1}\left(1 - \frac{\beta_{ij,n}}{\beta_{ij,1}}\right). \quad (6)$$

Here, the term $\sum_{i,j\in\{x,y\}} \frac{\hbar^2 k_i k_j}{2m_0}\beta_{ij,1}\left(1 - \frac{\beta_{ij,n}}{\beta_{ij,1}}\right)$ in Eq. (6) represents the difference in transverse kinetic energies in regions 1 and n. The term of $\frac{\hbar^2 k_i k_j}{2m_0}\beta_{ij,1}$ is identified as the kinetic energy of electron $\frac{m_0 v_e^2}{2\beta_{ij,1}}$ in region 1, where V_e is the gate electron phase velocity. A complete derivation can be found in Ref. [31].

The transmittance is analytically calculated by using the exponential- and Airy-wavefunction approach following Refs.[18, 23, 24]. Besides those approaches, the transmittance also computes numerically by employing the transfer matrix method (TMM) complying with Ref. [32].

The obtained transmittance is then applied to calculate the electron tunneling current by employing the following expression,

$$J_z = \frac{e\sum_l n_{vl} m_{dl}}{2\pi^2\hbar^3} \times \int_0^\infty T(E_z)kT \times \ln\left\{\frac{(1+\exp[(E_F - E_z)/kT])^\lambda}{1+\exp[(E_F - E_z - (eV_{ox} - \Delta))/kT]}\right\} dE_z, \quad (7)$$

where k is the Boltzmann constant, T is the temperature, n_{vl} is the valley degeneracy of Si, m_{dl} is the density of states mass of Si, E_F is the Fermi energy of the TiN_x gate, $\lambda = m_{tm}/m_{ts}$ is the ratio between the transverse effective masses in the TiN_x gate and the silicon substrate, $m_{ts} = \sum_l n_{vl} m_{dl}$, and $T(E_z)$ is the transmittance calculated using either the exponential- or the Airy-wavefunction approach or the TMM. The tunneling current in Eq. (7) is easily evaluated by using the Gauss–Laguerre Quadrature method[33].

3. Calculated results and discussion

In order to calculate the electron transmittance and tunneling current in the $TiN_x/HfO_2/SiO_2$/p-Si(100) MOS capacitor, the following parameters were used: Φ_a = 1.5 eV, Φ_b = 3.34 eV, d_1 = 1 nm, d_2 = 7.4 nm, κ_a = 25, κ_b = 3.9, $m_2 = 0.11m_0$, $m_3 = 0.8m_0$, and Δ = 0.53 eV[34–38]. The effective oxide thickness (EOT) of the 6.4 nm-thick HfO_2 layer, which is given by $(\kappa_b/\kappa_a)(d_2 - d_1)$, is about 1 nm. There are six equivalent valleys in the conduction band of Si(100) which are divided into three groups of valleys with the tensor elements α_{ij}, as shown in Table 1[39–41].

Figure 2 presents the electron transmittance as a function of energy of an electron in valley 1 (V1) for the gate electron phase velocity v_e of 1 × 10^5 m/s. The electron effective mass of TiN_x for the composition of 50% nitrogen of $3.1m_0$[12] was used in the calculation. It can be seen that the transmittances calculated by using the exponential- and Airy-wavefunction approaches and the TMM are a match for electron energies less than 3 eV, while for higher energies only the transmittances calculated under the Airy-wavefunction approach deviate insignificantly from those computed by the TMM. Moreover, the exponential-wavefunction approach gives an unphysical result in which the transmittance is higher than one for electron energies in the range of 4 to 10 eV (see the inset). These results imply that the exponential wavefunction is not appropriate in calculating the transmittance of a high energy electron.

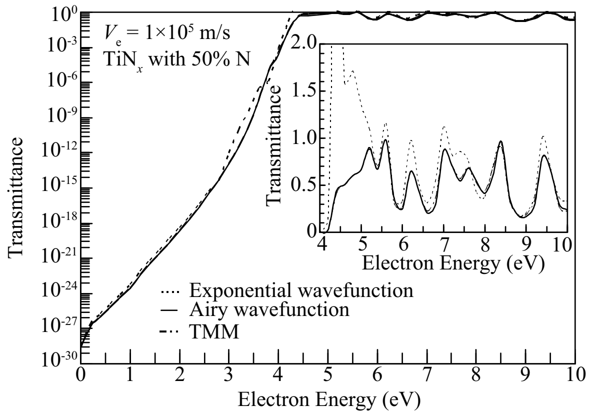

Fig. 2. Electron energy dependence of transmittance of an electron in valley 1 (V1) in which the gate electron phase velocity is 1 × 10^5 m/s.

Table 1. Tensor elements α_{ij} of Si(100).

Valley	Si(100)		
V1	1.02	0	0
	0	5.26	0
	0	0	5.26
V2	5.26	0	0
	0	1.02	0
	0	0	5.26
V3	5.26	0	0
	0	5.26	0
	0	0	1.02

The tunneling current in the $TiN_x/HfO_2/SiO_2$/p-Si(100) MOS capacitor as a function of oxide voltage is demonstrated in Fig. 3. It is found that the tunneling process from the metal gate to the silicon substrate does not happen for the oxide voltages lower than 0.53 V, as explained in Fig. 1(a). The tunneling currents increase as the oxide voltage increases. This can be understood from the fact that by applying a voltage to the barrier, the potential barrier in the right side is lowered, as shown in Fig. 1. Consequently, the effective height of the potential barrier is decreased so that the tunneling current is enhanced. It is also found that only the tunneling currents evaluated by applying the Airy-wavefunction approach match those obtained with the TMM. Again, these results give evidence that the Airy-wavefunction approach is better than the exponential-wavefunction approach.

Since the Airy-wavefunction approach is superior to the exponential-wavefunction approach, the Airy-wavefunction approach was then employed to calculate the tunneling current for several compositions of TiN_x metal gate, as presented in Fig. 4. The electron effective masses of TiN_x are $1.7m_0$, $2.4m_0$, $2.5m_0$, and $3.1m_0$ for 58%, 57%, 56%, and 50% nitrogen concentrations, respectively, and Reference [12] was used in the calculation. It is found that the tunneling current density decreases with increasing titanium concentration. This is because the effective height of the potential barrier is enhanced

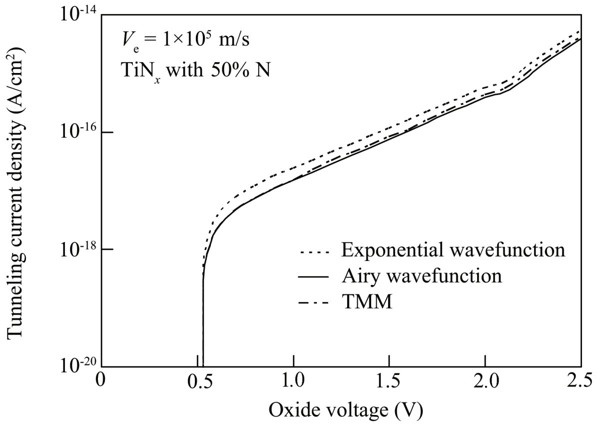

Fig. 3. Tunneling current as a function of oxide voltage for the gate electron phase velocity of 1×10^5 m/s.

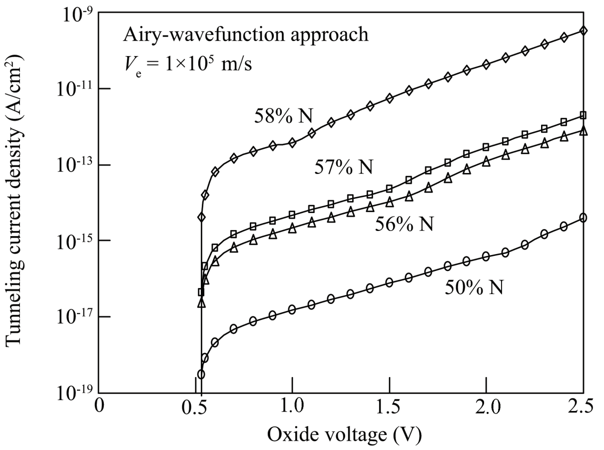

Fig. 4. Electron tunneling current density in the MOS capacitor for several nitrogen compositions of TiN_x calculated using the Airy-wavefunction approach.

by the increase in the electron effective mass of the TiN_x metal gate, as shown in Eq. (6). The transmittance then decreases and the tunneling current density therefore reduces. This means that the alteration in the titanium concentration of the TiN_x metal gate causes the change in the tunneling current.

In order to know the effect of mass anisotropy on the tunneling current in the MOS capacitor, we compared the tunneling currents calculated with the anisotropic and isotropic masses by including the transverse-longitudinal kinetic energy coupling under the Airy-wavefunction approach. The results are given in Fig. 5. It is shown that the calculated tunneling current under the anisotropic mass is about five orders of magnitude lower than that obtained under the isotropic mass. This means that the mass anisotropy significantly affects the tunneling current in the MOS capacitor and the mass anisotropy is therefore not negligible.

4. Conclusions

An analytical expression of electron transmittance and tunneling current in the $TiN_x/HfO_2/SiO_2$/p-Si(100) MOS capacitor under a negative bias voltage applied to the TiN_x gate have been derived. The electron transmittance and tunneling current are derived by employing exponential- and Airy-wavefunction

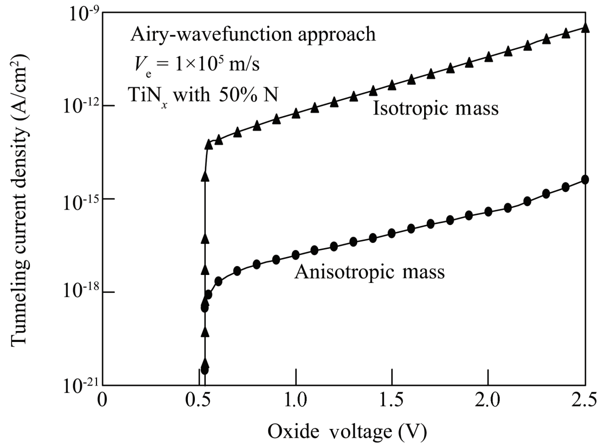

Fig. 5. Tunneling currents calculated by employing the Airy-wavefunction approach under the isotropic and anisotropic masses.

approaches and examined by utilizing a transfer matrix method (TMM). It has been found that the transmittances calculated by utilizing the exponential- and Airy-wavefunction approaches and the TMM are the same for low electron energies (less than 3 eV), while for higher electron energies only the tunneling currents computed under the Airy-wavefunction approach match those obtained under the TMM. It has also been found that for all range of oxide voltages only the tunneling currents evaluated by using the Airy-wavefunction approach fit those obtained with the TMM. The Airy-wavefunction approach is therefore better than the exponential-wavefunction one to model analytically tunneling processes in the MOS capacitor. In addition, the tunneling current density decreases with increasing titanium concentration of the TiN_x metal gate because the electron effective mass of TiN_x increases with the decrease in nitrogen concentration. Moreover, the mass anisotropy must be taken into account because the tunneling current calculated under the anisotropic mass significantly differs from that obtained under the isotropic mass.

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