Simulation of Electron Transmittance and Tunneling Current in a Metal-Oxide-Semiconductor Capacitor with a High-K Dielectric Stack of HfO₂ and SiO₂ 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 a metal-oxide-semiconductor (MOS) capacitor with a high dielectric constant (high-K) oxide stack of HfO₂ and SiO₂ and a negative bias applied to the metal gate were derived. Exponential- and Airy-wavefunction approaches were employed in deriving analytically the electron transmittance and tunneling current. A numerical approach based on a transfer matrix method was used as a standard to evaluate the analytical approaches. It was found that the transmittances obtained under the exponential- and Airy-wavefunction approaches and the TMM are matching for low electron energies, while for higher energies only the transmittances calculated by employing the Airy- wavefunction approach is the same as those computed by using the TMM. It was also found that the tunneling currents calculated by using the exponential- and the Airy-wavefunction approaches and the TMM are equal for low oxide voltages (lower than 0.5 V), while for higher oxide voltages only the tunneling currents computed under the Airy-wavefunction approach fit those obtained under the TMM. Therefore, the Airy-wavefunction approach provides a better analytical model to tunneling processes in the MOS capacitor.

Keywords: Airy wavefunction, Current, Exponential wavefunction, Transmittance, Tunneling

1. Introduction

Many theoretical and experimental investigations have been carried out to study electron tunneling processes in heterostructures since five decades ago¹⁻⁶. One of the heterostructures is a metal-oxide-semiconductor (MOS) capacitor in which its feature sizes are aggressively scaled-down to nanoscale dimensions in order to enhance its performance^{7,8}. At present, the oxide layer of MOS capacitor is a stack of SiO₂ and a high dielectric constant (high-K) material so that the stand-by power consumption of the capacitor, which originates from a leakage current due to electrons tunneling through the oxide stack, is reduced^{9,10}.

Basically, the behavior of electrons tunneling through the oxide layer is studied by solving the Schrödinger equation analytically or numerically. Among analytical approaches, an exponential-wavefunction approach has been applied to calculate an electron direct transmittance and tunneling time in an Si/SiO₂/Si heterostructure¹¹. Very recently, an Airy-wavefunction approach has been employed in computing the tunneling times and currents in MOS capacitors and it has been found that the tunneling times and currents obtained by using this approach differ from those achieved under the exponential-wavefunction one^{12,13}. However, it has not been concluded which analytical approach is appropriate in describing the tunneling processes.

In this paper, we report electron transmittance and tunneling current in an Al/HfO₂/SiO₂/p-Si MOS capacitor evaluated analytically by utilizing the exponential- and Airy-wavefunctions approaches. A

transfer matrix method (TMM), which is a numerical method to solve the Schrödinger equation for various problems¹⁴⁻²¹, is used to examine the analytical approaches. Calculated results are discussed thoroughly.

2. Theoretical Model

Figure 1(a) shows the schematic energy diagram of an Al/HfO₂/SiO₂/p-Si MOS capacitor in a flatband condition. Here, ϕ_m is the metal work function, χ is the electron affinity of Si, E_c and E_v are the conduction and valence bands of Si, respectively, and E_F is the Fermi level of Si, and $E_{g,a}$, $E_{g,b}$, and $E_{g,Si}$ are the band gaps of HfO₂, SiO₂, and Si, respectively. Other parameters are Φ_a and Φ_b , which are the conduction band discontinuities of Si/HfO₂ and Si/SiO₂, respectively, and d_1 and (d_2-d_1) , which are the thicknesses of HfO₂ and SiO₂, respectively. Under the application of a negative voltage to the Al gate, electrons originating from the Al gate tunnel through the high-K dielectric stack and then sink into the p-type silicon substrate. The potential profile due to the negative gate voltage as demonstrated in Fig. 1(b) is easily obtained by using basic electrostatics and it can be mathematically expressed as

$$V(z) = \begin{cases} 0 & z < 0 \\ (\Phi_a + \Delta) - \varepsilon_b p z & 0 \leq z < d_1 \\ (\Phi_b + \Delta) - \varepsilon_b p d_1 - \varepsilon_a p (z - d_1) & d_1 \leq z < d_2 \\ \Delta - \varepsilon_b p d_1 - \varepsilon_a p d_2 & z \geq d_2, \end{cases} \quad (1)$$

where $p = \frac{eV_{ox}}{\varepsilon_a\delta_2 + \varepsilon_b d_1}$, e is the electronic charge, V_{ox} is the oxide voltage, which is the voltage across the high-K gate stack, $\varepsilon_a = \varepsilon_0 K_a$ and $\varepsilon_b = \varepsilon_0 K_b$ are the permittivities of HfO_2 and SiO_2 , respectively, and $\delta_2 = d_2 - d_1$. The constants ε_0 is the permittivity in vacuum, K_a and K_b are the dielectric constants of HfO_2 and SiO_2 , respectively.

Figure 1(a) The energy band diagram of an Al/HfO2/SiO2/p-Si MOS capacitor in a flatband condition and (b) potential profile in the z-direction under a negative bias voltage applied to the Al gate.

The behavior of an electron in the Al/HfO2/SiO2/Si(100) MOS capacitor is described by the Schrödinger equation²²⁾

$$-\frac{\hbar^2}{2m^*} \frac{d^2\Psi}{dz^2} + U(z)\Psi(z) = E\Psi(z), \quad (2)$$

where m^* is the effective mass of electron, $\hbar$ is the reduced Planck constant, E and $\Psi(z)$ are the electron energy and wavefunction, respectively, and $U(z)$ is the potential profile given by Eq. (1).

2. 1. Transmittance under the Exponential-Wavefunction Approach

Electron wavefunctions as general solutions of the Schrödinger equation in Eq. (2) with a trapezoidal

potential barrier can be expressed as linear combinations of exponential functions¹¹⁾. For the potential profile given by Eq. (1), the electron wavefunctions in all regions are written as

$$\Psi(z) = \begin{cases} A \exp(ik_1 z) + B \exp(-ik_1 z) & z < 0 \\ C \exp\left(\int_0^z k_2(z) dz\right) + D \exp\left(-\int_0^z k_2(z) dz\right) & 0 \leq z < d_1 \\ E \exp\left(\int_{d_1}^z k_3(z) dz\right) + F \exp\left(-\int_{d_1}^z k_3(z) dz\right) & d_1 \leq z < d_2 \\ G \exp(ik_4 z) & z \geq d_2 \end{cases} \quad (3)$$

where A is the incident wave amplitude, C and G are the transmitted wave amplitudes, and B and D are the reflected wave amplitudes. The wavenumbers in each region k_1 , k_2 , k_3 , and k_4 are respectively described by

$$k_1 = \left(\frac{2m_1(E_z - U_1(z))}{\hbar^2} \right)^{\frac{1}{2}} \quad z < 0 \text{ (region 1)}, \quad (4.a)$$

$$k_2(z) = \left(\frac{2m_2(U_2(z) - E_z)}{\hbar^2} \right)^{\frac{1}{2}} \quad 0 \leq z < d_1 \text{ (region 2)}, \quad (4.b)$$

$$k_3(z) = \left(\frac{2m_3(U_3(z) - E_z)}{\hbar^2} \right)^{\frac{1}{2}} \quad d_1 \leq z < d_2 \text{ (region 3)}, \quad (4.c)$$

$$k_4 = \left(\frac{2m_4(E_z - U_4(z))}{\hbar^2} \right)^{\frac{1}{2}} \quad z \geq d_2 \text{ (region 4)}, \quad (4.d)$$

where m_i and $U_i(z)$ ($i = 1, 2, 3, 4$) are the electron effective mass and the potential energy in region i , respectively.

Noting that the boundary conditions of BenDaniel-Duke²³⁾ at $z=0$, $z=d_1$, and $z=d_2$ hold, namely,

$$\Psi_1(z=0^-) = \Psi_2(z=0^+), \quad \frac{1}{m_1} \frac{d\Psi_1}{dz} \Big|_{z=0^-} = \frac{1}{m_2} \frac{d\Psi_2}{dz} \Big|_{z=0^+}, \quad (5.a)$$

$$\Psi_2(z=d_1^-) = \Psi_3(z=d_1^+), \quad \frac{1}{m_2} \frac{d\Psi_2}{dz} \Big|_{z=d_1^-} = \frac{1}{m_3} \frac{d\Psi_3}{dz} \Big|_{z=d_1^+}, \quad (5.b)$$

$$\Psi_3(z=d_2^-) = \Psi_4(z=d_2^+), \quad \frac{1}{m_3} \frac{d\Psi_3}{dz} \Big|_{z=d_2^-} = \frac{1}{m_4} \frac{d\Psi_4}{dz} \Big|_{z=d_2^+}, \quad (5.c)$$

it is easily obtained the relation between the constants G and A , which is given by

$$f = \frac{G}{A} = \frac{2ik_1}{m_1} (b_1^2 - b_2^2) \frac{k_3(d_2)}{k_3(d_1)} \frac{e^{-ik_4 d_2}}{M + N}. \quad (6)$$

Here,

$$M = a_1(b_1 b_3 \exp(-\alpha) \exp(\beta) - b_2 b_4 \exp(-\alpha) \exp(-\beta)), \quad (7.a)$$

$$N = a_2(b_1 b_4 \exp(\alpha) \exp(-\beta) - b_2 b_3 \exp(\alpha) \exp(\beta)) \quad (7.b)$$

$$a_1 = \left(\frac{ik_1}{m_1} + \frac{k_2(0)}{m_2} \right), \quad a_2 = \left(\frac{ik_1}{m_1} + \frac{k_2(0)}{m_2} \right). \quad (7.c)$$

$$b_1 = \left(\frac{k_3(d_1)}{m_3} - \frac{k_2(d_1)}{m_2} \right), \quad b_2 = \left(\frac{k_3(d_1)}{m_3} + \frac{k_2(d_1)}{m_2} \right). \quad (7.d)$$

$$b_3 = \left(\frac{k_3(d_2)}{m_3} - \frac{ik_4}{m_4} \right), \quad b_4 = \left(\frac{k_3(d_2)}{m_3} + \frac{ik_4}{m_4} \right). \quad (7.e)$$

$$\alpha = \int_0^{d_1} k_2(z) dz, \quad \beta = \int_{d_1}^{d_2} k_3(z) dz. \quad (7.f)$$

The transmittance T can be written as²²⁾

$$T = \frac{k_4}{k_1} f \cdot f^*, \quad (8)$$

where f^* is the complex conjugate of f .

2.2. Transmittance under the Airy-Wavefunction Approach

Other solutions of the Schrödinger equation in Eq. (2) with a trapezoidal potential barrier can also be expressed as linear combinations of Airy functions^{12,13)}. The electron wavefunctions in all regions for the potential profile given by Eq. (2) can also be written as

$$\Psi(z) = \begin{cases} A \exp(ik_1 z) + B \exp(-ik_1 z) & z \leq 0 \\ C \text{Ai}(\varepsilon(z)) + D \text{Bi}(\varepsilon(z)) & 0 < z \leq d_1 \\ E \text{Ai}(\eta(z)) + F \text{Bi}(\eta(z)) & d_1 < z < d_2 \\ G \exp(ik_4 z) & z \geq d_2, \end{cases} \quad (9)$$

where k_1 and k_4 are the the same as those given in Eqs. (4.a) and (4.d), respectively. The terms $\varepsilon(z)$ and $\eta(z)$ are the arguments of Airy functions Ai and Bi in regions 2 and 3, respectively, which are described by

$$\varepsilon(z) = \left(\frac{2m_0}{\hbar^2} \frac{1}{\alpha_{zz,2}} \kappa_b p \right)^{\frac{1}{3}} \left(-z + \frac{(\Phi_a + \Delta) - E_{z,1}}{\kappa_b p} \right) \quad (10)$$

$$\eta(z) = \left(\frac{2m_0}{\hbar^2} \frac{1}{\alpha_{zz,3}} \kappa_a p \right)^{\frac{1}{3}} \left(-z + \frac{(\Phi_b + \Delta) - E_{z,1}}{\kappa_a p} + \frac{d_1(\kappa_a - \kappa_b)}{\kappa_a p} \right) \quad (11)$$

Applying the boundary conditions in Eq. (5), the relation between the constants G and A in Eq. (9) is given by

$$f = \frac{G}{A} = \frac{2u_1 c_9 (c_3 c_8 - c_6 c_7)}{c_1 c_{10} (c_2 c_3 - c_5 c_6) - c_1 c_{11} (c_2 c_7 - c_5 c_8)} e^{-ik_4 d_2}. \quad (12)$$

Here,

$$u_1 = i \frac{k_1}{m_1}, \quad (13.a)$$

$$w_1 = - \left(\frac{2m_0}{\hbar^2} \frac{1}{\alpha_{zz,2}} \kappa_b p \right)^{\frac{1}{3}}, \quad (13.b)$$

$$w_2 = - \left(\frac{2m_3}{\hbar^2} \kappa_a p \right)^{\frac{1}{3}}, \quad (13.c)$$

$$c_1 = \frac{w_2}{m_3} \text{Ai}'(\eta(d_1)) \text{Bi}(\eta(d_1)) - \frac{w_2}{m_3} \text{Bi}'(\eta(d_1)) \text{Ai}(\eta(d_1)), \quad (13.d)$$

$$c_2 = \frac{w_2}{m_3} \text{Ai}'(\eta(d_2)) - u_4 \text{Ai}(\eta(d_2)), \quad (13.e)$$

$$c_3 = \frac{w_2}{m_3} \text{Bi}'(\eta(d_1)) \text{Bi}(\varepsilon(d_1)) - \frac{w_1}{m_2} \text{Bi}'(\varepsilon(d_1)) \text{Bi}(\eta(d_1)), \quad (13.f)$$

$$c_5 = \frac{w_2}{m_3} \text{Bi}'(\eta(d_2)) - u_4 \text{Bi}(\eta(d_2)), \quad (13.g)$$

$$c_6 = \frac{w_2}{m_3} \text{Ai}'(\eta(d_1)) \text{Bi}(\varepsilon(d_1)) - \frac{w_1}{m_2} \text{Bi}'(\varepsilon(d_1)) \text{Ai}(\eta(d_1)), \quad (13.h)$$

$$c_7 = \text{Ai}(\varepsilon(d_1)) \frac{w_2}{m_3} \text{Bi}'(\eta(d_1)) - \text{Bi}(\eta(d_1)) \frac{w_1}{m_2} \text{Ai}'(\varepsilon(d_1)), \quad (13.i)$$

$$c_8 = \frac{w_2}{m_3} \text{Ai}'(\eta(d_1)) \text{Ai}(\varepsilon(d_1)) - \frac{w_1}{m_2} \text{Ai}'(\varepsilon(d_1)) \text{Ai}(\eta(d_1)), \quad (13.j)$$

$$c_9 = \frac{w_2}{m_3} \text{Ai}'(\eta(d_2)) \text{Bi}(\eta(d_2)) - \frac{w_2}{m_3} \text{Bi}'(\eta(d_2)) \text{Ai}(\eta(d_2)), \quad (13.k)$$

$$c_{10} = u_1 \text{Ai}(\varepsilon(0)) + \frac{w_1}{m_2} \text{Ai}'(\varepsilon(0)), \quad (13.l)$$

$$c_{11} = u_1 \text{Bi}(\varepsilon(0)) + \frac{w_1}{m_2} \text{Bi}'(\varepsilon(0)). \quad (13.m)$$

The transmittance T can be obtained by substituting Eq. (12) into Eq. (8).

2.3 Transmittance under the Transfer Matrix Method (TMM)

The TMM is based on dividing the domain of the solution into N segments as illustrated in Fig. 2 in which each segment of the potential energy, U_j , is constant. The time-independent electron wavefunction in each region is¹⁵⁾

$$\Psi_1(z) = \exp(i\delta_1 z) + B_1 \exp(-i\delta_1 z) \quad z \leq 0, \quad (14.a)$$

$$\Psi_j(z) = A_j \exp(\delta_j z) + B_j \exp(-\delta_j z) \quad 0 < z < d_2, \quad (14.b)$$

$$\Psi_N(z) = A_N \exp(i\delta_N z) \quad z \geq d_2, \quad (14.c)$$

where δ_1 and δ_N are the wavenumbers that are the same as those given in Eqs. (4.a) and (4.d), respectively, A_j and B_j are the amplitudes, $\delta_j = (2m_j(U_j - E)/\hbar^2)^{1/2}$ is the wavenumber, m_j is the electron effective mass, and U_j is the constant potential in the j^{th} segment for $1 < j < N$.

Figure 2. The trapezoidal potential barrier is divided into $N-2$ segments

Applying the boundary condition¹⁷⁾ at the interface of $(j-1)^{\text{th}}$ and j^{th} segments,

$$\Psi_{j-1}(z = z_{j-1}^-) = \Psi_j(z = z_{j-1}^+), \quad (15)$$

$$\frac{1}{m_{j-1}} \frac{d\Psi_{j-1}}{dz} \Big|_{z=z_{j-1}^-} = \frac{1}{m_j} \frac{d\Psi_j}{dz} \Big|_{z=z_{j-1}^+}$$

it is easily obtained the following matrix equations

$$\begin{pmatrix} 1 \\ B_1 \end{pmatrix} = M_{12} M_{23} M_{34} \dots M_{N-1N} \begin{pmatrix} A_N \\ 0 \end{pmatrix}, \quad (16)$$

where M_{ij+1} is a matrix relating A_j and B_j with A_{j+1} and B_{j+1} .

Expressing Eq. (16) as

$$\begin{pmatrix} 1 \\ B_1 \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \begin{pmatrix} A_N \\ 0 \end{pmatrix}, \quad \text{the term } f \text{ becomes}$$

$$f = A_N = \frac{1}{g_{11}}. \quad (17)$$

Substituting Eq. (17) into Eq. (8), we can obtain the transmittance T .

2.3 Calculation of Electron Tunneling Current

The electron tunneling current is calculated by employing the following expression²⁴⁾

$$J = \frac{e \sum n_{vi} m_{dl}}{2\pi^2 \hbar^3} \times \int_0^\infty T(E) kT \ln \left\{ \frac{1 + \exp[(E_F - E_z)/kT]}{1 + \exp[(E_F - E_z - V)/kT]} \right\} dE_z \quad (18)$$

where e is the electronic charge, k is the Boltzmann constant, n_{vi} is the valley degeneracy of Si, m_{dl} is the density of states mass of Si, E_F is the Fermi energy of Al gate, and T is the transmittance calculated using either the exponential or exponential- and Airy-wavefunctions or TMM. The tunneling current in Eq. (18) is easily evaluated by using the Gauss-Laguerre Quadrature method²⁵⁾.

3. Calculated Results and Discussion

The electron transmittance and tunneling current in the Al/HfO₂/SiO₂/p-Si(100) MOS capacitor were calculated by using Eqs. (8) and (18), respectively. The parameters used in calculating the transmittance and tunneling current were the following: $\Phi_a = 1.5$ eV, $\Phi_b = 3.1$ eV, $d_1 = 1$ nm, $d_2 = 7.4$ nm, $K_a = 25$, $K_b = 3.9$, $m_1 = m_0$, $m_2 = 0.17 m_0$, and $m_3 = 0.5 m_0$.^{26,27)} The effective oxide thickness (EOT) of the 6.4 nm-thick HfO₂ layer, which is given by $(K_b/K_a)(d_2 - d_1)$, is about 1 nm. The Si(100) surface has two possible values of m_z in the six ellipsoids of conduction band energy. The two ellipsoids (the valley L) in the z axis have $m_z = 0.916 m_0$, $n_v = 2$, and $m_d = 0.19 m_0$ and the four ellipsoids in the x - y plane (the valley H) have $m_z = 0.19 m_0$, $n_v = 4$, and $m_d = 0.417 m_0$, where m_0 is the free electron mass.²⁴⁾

Figure 3. The energy dependence of transmittance of an electron in the valley L.

Figure 3 presents the electron transmittance as a function of energy of an electron in the valley L, which were calculated by employing the exponential- and Airy-wavefunction approaches and the TMM. It can be seen that the transmittances are identical for low electron energies (less than 1 eV). On the other hand, for higher energies, only the transmittances calculated by using the Airy-wavefunction approach is

the same as those evaluated by employing 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 3 to 5 eV. These findings imply that the use of exponential wavefunctions in calculating the transmittance of a high energy electron is not appropriate.

Figure 4. The energy dependence of transmittance of an electron in the valley H.

The energy dependence of the electron transmittance for the valley H is depicted in Figure 4. The results for an electron in the valley H are the same as those in the valley L. The transmittances obtained by using the exponential- and Airy-wavefunction approaches and the TMM are matching for low electron energies (less than 1 eV). For higher energies, only the transmittances computed by using the Airy-wavefunction approach is the same as those evaluated by employing the TMM. These assert that the Airy-wavefunction approach is more accurate than the exponential- wavefunction one.

Figure 5. The electron tunneling current versus oxide voltage.

The tunneling current in the Al/HfO₂/SiO₂/p-Si(100) MOS capacitor as a function of oxide voltage is demonstrated in Figure 5. The tunneling currents increase with the oxide voltage. This can be understood from the fact that the potential barrier is lowered by the oxide voltage as shown in Figure 1. An increase of the oxide voltage decreases the potential

barrier height and then increases the transmittance. Therefore, the tunneling current is enhanced. It is also found that the tunneling currents obtained by employing the exponential- and the Airy-wavefunction approaches and the TMM are equivalent for low oxide voltages (lower than 0.5 V), while for higher oxide voltages only the tunneling currents calculated by using the Airy-wavefunction approach fit those obtained with the TMM. Again, these results state that the Airy-wavefunction approach is better than the exponential-wavefunction one.

4. Conclusions

We have derived analytical expressions of electron transmittance and tunneling current in an Al/HfO₂/SiO₂/p-Si(100) MOS capacitor under a negative bias applied to the Al gate. Exponential- and Airy-wavefunction approaches have been employed in deriving analytically the electron transmittance and tunneling current. A transfer matrix method has been utilized to examine the analytical approaches. It has been found that the transmittances calculated by employing the exponential- and Airy-wavefunction approaches and the TMM are identical for low electron energies (less than 1 eV). For higher energies, only the transmittances obtained by using the Airy-wavefunction approach is the same as that computed by employing the TMM. It has also been found that the tunneling currents calculated by using the exponential- and the Airy-wavefunction approaches and the TMM are the same for low oxide voltages (lower than 0.5 V), while for higher oxide voltages only the tunneling currents calculated by using the Airy-wavefunction approach match 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.

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