WKB approximation based formula for tunneling probability through a multi-layer potential barrier

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Abstract— **In this work, we present a theoretical derivation of the analytical formula for tunneling probability through an n-layer barrier basing on the Wentzel-Kramers-Brillouin (WKB) and the effective mass approximations. The accuracy of the derived formula is analysed by comparison with the transfer matrix method (TMM). The effect of the electric charge distribution in a stack on the tunnel current is considered.**

Keywords: MOS structures, modelling, tunneling

I. INTRODUCTION

Gate stacks in the advanced MOSFETs can consist of two or even more layers to fulfil requirements for high quality of the interface with the semiconductor substrate, high overall electric permittivity, thermal stability and a desirable work-function of the gate material. A multi-layer structure of a gate stack complicates theoretical simulations of the tunnel leakage. Although the transfer matrix method (TMM) [1] can serve as a universal computational tool for calculation of the tunneling probability for any shape of the barrier, analytical modelling always would be preferred. In [2], a formula for tunnelling through a single-layer barrier was derived basing on the WKB approximation. In [3], an analogous formula was presented in terms of the group velocities in the pre-exponential term called the correction factor, founding a lot of citations in the literature. In [4] and [5], analytical formulae for the double-layer and three-layer barriers were obtained after the use of asymptotic forms of the Airy functions in the exact expressions. In [5], basing on analogies for the single-, double- and three-layer barriers, an analytical formula for the *n*-layer barrier was postulated and checked by comparison with results of the TMM-based simulations. In this work, we present a theoretical derivation of the formula for an n-layer barrier basing on the WKB approximation and analyse its accuracy. Concluding that the formula does not change if the electric charges are built-in inside the gate stack, we exploit it to search the effect of the electric charge distribution in a stack on the tunnel current.

II. THEORY

Let us consider an electron hitting the barrier from the left side (Fig. 1) and use the WKB approximation for the wave functions in all the regions:

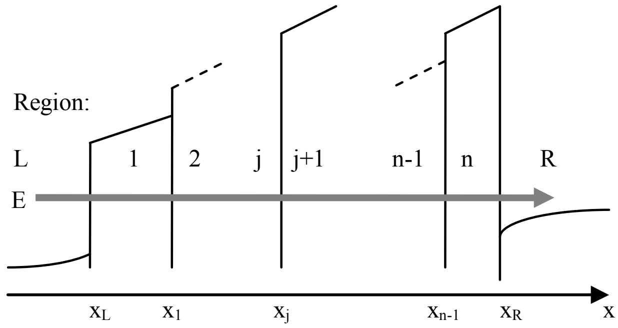


Figure 1. Energy diagram of an *n*-layer potential barrier.

- *L* – the left electrode:

$$\varphi_L = \frac{A_L}{\sqrt{k_L}}\exp\left(i\int_{x_L}^{x} k_L dx\right) + \frac{B_L}{\sqrt{k_L}}\exp\left(-i\int_{x_L}^{x} k_L dx\right) \tag{1}$$

- *j* = from 1 to *n* – the barrier layers:

$$\varphi_j = \frac{A_j}{\sqrt{\kappa_j}}\exp\left(-\int_{x_{j-1}}^{x} \kappa_j dx\right) + \frac{B_j}{\sqrt{\kappa_j}}\exp\left(\int_{x_{j-1}}^{x} \kappa_j dx\right) \tag{2}$$

- *R* – the right electrode:

$$\varphi_R = \frac{A_R}{\sqrt{k_R}}\exp\left(i\int_{x_R}^{x} k_R dx\right) + \frac{B_R}{\sqrt{k_R}}\exp\left(-i\int_{x_R}^{x} k_R dx\right) \tag{3}$$

where k_L and k_R are wave vectors in the outer regions and κ_j denotes the imaginary part of the wave vector in the *j*-th barrier layer for the direct tunneling regime.

Conditions for continuity of φ and $m^{-1}d\varphi/dx$ under the restriction:

$$\left|\frac{dk}{dx}\right| \langle\langle \left|k^2\right| \tag{4}$$

lead to equations expressed by means of the reverse transfer matrices R:

- for $x = x_L$ (matrix R_L):

$$\begin{bmatrix} A_L \\ B_L \end{bmatrix} = [R_L]\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} \tag{5}$$

where:

$$[R_L] = \frac{m_L}{2\sqrt{k_L\kappa_{1L}}}\begin{bmatrix} \left(\frac{k_L}{m_L} + i\frac{\kappa_{1L}}{m_1}\right) & \left(\frac{k_L}{m_L} - i\frac{\kappa_{1L}}{m_1}\right) \\ \left(\frac{k_L}{m_L} - i\frac{\kappa_{1L}}{m_1}\right) & \left(\frac{k_L}{m_L} + i\frac{\kappa_{1L}}{m_1}\right) \end{bmatrix} \tag{6}$$

- for $x = x_1$ to x_{n-1} (matrices R_j):

$$\begin{bmatrix} A_j \\ B_j \end{bmatrix} = [R_j]\begin{bmatrix} A_{j+1} \\ B_{j+1} \end{bmatrix} \tag{7}$$

where:

$$[R_j] = \frac{m_j}{2\sqrt{\kappa_{jx_j}\kappa_{(j+1)x_j}}}\begin{bmatrix} \left(\frac{\kappa_{jx_j}}{m_j} + \frac{\kappa_{(j+1)x_j}}{m_{j+1}}\right)e^{S_j} & \left(\frac{\kappa_{jx_j}}{m_j} - \frac{\kappa_{(j+1)x_j}}{m_{j+1}}\right)e^{S_j} \\ \left(\frac{\kappa_{jx_j}}{m_j} - \frac{\kappa_{(j+1)x_j}}{m_{j+1}}\right)e^{-S_j} & \left(\frac{\kappa_{jx_j}}{m_j} + \frac{\kappa_{(j+1)x_j}}{m_{j+1}}\right)e^{-S_j} \end{bmatrix} \tag{8}$$

- for $x = x_R$ (matrix R_R):

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = [R_R]\begin{bmatrix} A_R \\ B_R \end{bmatrix} \tag{9}$$

where:

$$[R_R] = \frac{m_n}{2\sqrt{\kappa_{nR}k_R}}\begin{bmatrix} \left(\frac{\kappa_{nR}}{m_n} - i\frac{k_R}{m_R}\right)e^{S_n} & \left(\frac{\kappa_{nR}}{m_n} + i\frac{k_R}{m_R}\right)e^{S_n} \\ \left(\frac{\kappa_{nR}}{m_n} + i\frac{k_R}{m_R}\right)e^{-S_n} & \left(\frac{\kappa_{nR}}{m_n} - i\frac{k_R}{m_R}\right)e^{-S_n} \end{bmatrix} \tag{10}$$

and:

$k_L=k_L(x_L)$, $k_{1L}=k_1(x_L)$, $k_{jx_j}=k_j(x_j)$, $k_{nR}=k_n(x_R)$, $k_R=k_R(x_R)$,

$$S_j = \int_{x_{j-1}}^{x_j} \kappa_j dx \tag{11}$$

If all terms containing $exp(-S_j)$ are neglected for $S_j >> 1$ and B_R is set to zero, then:

$$A_L \approx R_{11L}\prod_{i=1}^{n-1} R_{11i}R_{11R}A_R \tag{12}$$

Tunneling probability, which is defined as the ratio of the forward flowing probability currents in the outer regions R and L, takes the form:

$$P_{WKB} \approx \frac{\frac{i\hbar}{2m_R}\left(\varphi_R^*\nabla\varphi_R - \varphi_R\nabla\varphi_R^*\right)}{\frac{i\hbar}{2m_L}\left(\varphi_L^*\nabla\varphi_L - \varphi_L\nabla\varphi_L^*\right)} \approx \frac{\frac{\hbar}{m_R}\left|A_R\right|^2}{\frac{\hbar}{m_L}\left|A_L\right|^2} = P_0 \exp\left[-2\int_{x_L}^{x_R}\kappa(x)dx\right] \tag{13}$$

where P_0 is the energy-dependent pre-exponential term:

$$P_0 = \frac{16\frac{k_L}{m_L}\frac{\kappa_{1L}}{m_1}\frac{\kappa_{nR}}{m_n}\frac{k_R}{m_R}}{\left[\left(\frac{k_L}{m_L}\right)^2 + \left(\frac{\kappa_{1L}}{m_1}\right)^2\right]\left[\left(\frac{\kappa_{nR}}{m_n}\right)^2 + \left(\frac{k_R}{m_R}\right)^2\right]} \times$$

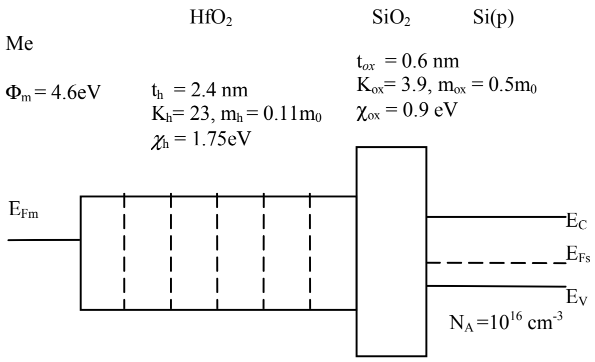
$$\times\prod_{j=1}^{n-1}\left[\frac{4\frac{\kappa_{jx_j}}{m_j}\frac{\kappa_{(j+1)x_j}}{m_{j+1}}}{\left(\frac{\kappa_{jx_j}}{m_j} + \frac{\kappa_{(j+1)x_j}}{m_{j+1}}\right)^2}\right] \tag{14}$$

III. DISCUSSION

The term in the product for the j-th interface of the stack disappears if κ/m is continuous, i.e.

$$\frac{\kappa_j}{m_j} = \frac{\kappa_{j+1}}{m_{j+1}} \tag{15}$$

This proves that the pre-exponential term does not change if volume traps are located in the stack, provided they do not scatter electrons. The effect of charges distributed in the stack on the tunnel current can be easily included by dividing the stack into clusters with charges between them, as shown in Fig. 2. The three considered charge distributions correspond to the same effective oxide charge Q_{eff}= 4.2x10^{12}cm^{-2}, i.e. to the same surface potential in the substrate at a given gate voltage.



	Q_1	Q_2	Q_3	Q_4	Q_5	Q_6	Q_7
Stack A	0	0	0	0	0	0	$4.2\cdot10^{12}$
Stack B	0	0	0	0	0	10^{13}	0
Stack C	$3\cdot10^{12}$	$3\cdot10^{12}$	$3\cdot10^{12}$	$3\cdot10^{12}$	$3\cdot10^{12}$	$3\cdot10^{12}$	0

Figure 2. The simulated gate stacks.

Fig. 3 shows the energy dependence of the tunneling probability across the Stack A at V_G = 1V for three cases of calculations:

- *P_TMM*: transfer matrix method,
- *exp(-2S)*: only the exponential term of the derived formula (13),
- *P_WKB*: full WKB-based formula (13) (14),

and for two values of the effective mass in silicon. The exponential term does not depend on the effective mass in the outer electrodes.

The current-voltage (*I-V*) characteristics for the three considered charge distributions are presented in Fig. 4. The trapped charges influence effectively the *I-V* dependence only in the depletion range. The positive charge located across the high-K layer or at the high-K/SiO_2 interface give higher tunnel current than the equivalent charge at the substrate interface. Although the assumed charge density is high, the effect of its distribution on the tunnel current is not significantly strong due to high value of the gate stack capacitance caused by low equivalent oxide thickness.

IV. Conclusions

Fig. 3 illustrates a very good accuracy of the WKB-based formula for the direct regime of tunneling. The use of the simplified form of the WKB-based formula, i.e., without the pre-exponential term, leads to significant inaccuracy of modelling. The pre-exponential term does not change if the discrete charges are incorporated in the volume of the gate stack materials provided the ratio κ/m is continuous.

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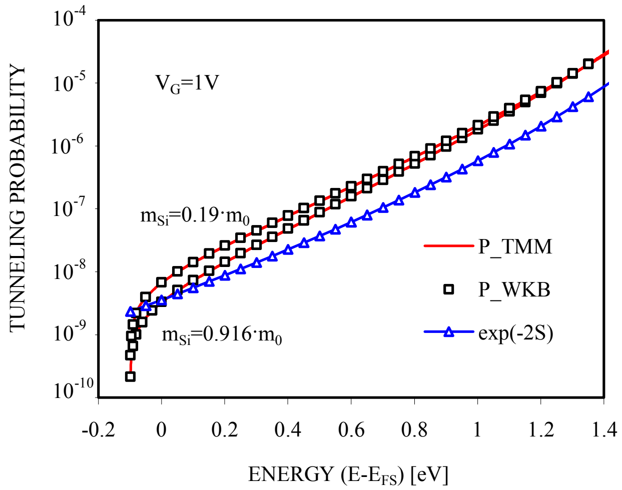

Figure 3. Energy dependence of the tunneling probability.

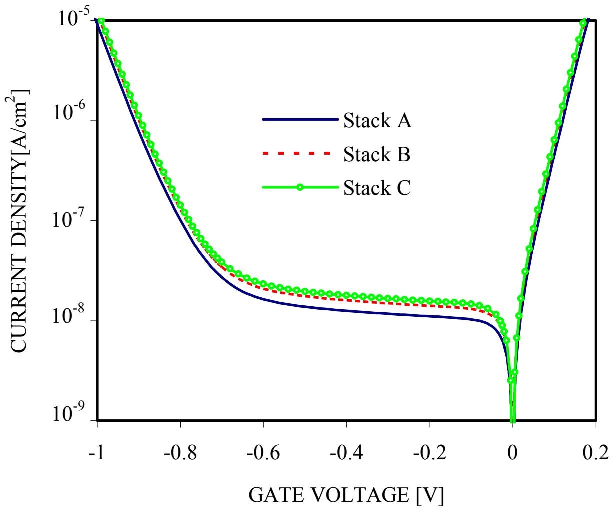

Figure 4. Charge distribution effect on the tunneling current.

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