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

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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 tunnelling 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 the 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 the stack on the tunnel current.

THEORY

Fig. 1 shows the energy band diagram of the multi-layer barrier to define the used notation.

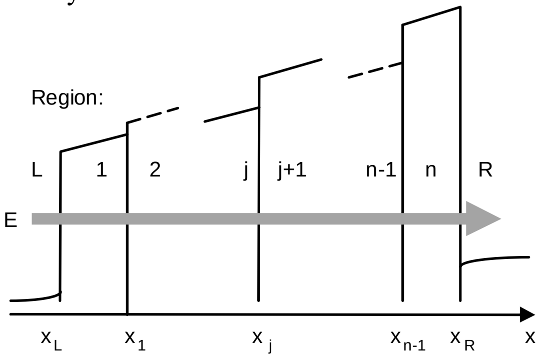

Fig. 1. Energy diagram of the n-layer potential barrier.

Let us consider an electron hitting the barrier from the left side and use the WKB approximation for the wave functions in all the regions: L – the left electrode, j = from 1 to n – the barrier layers, and R – the right electrode:

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

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

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

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 tunnelling regime. Conditions for continuity of φ and $m^{-1}\mathrm{d}\varphi/\mathrm{d}x$ under the restriction $|\mathrm{d}k/\mathrm{d}x| << |k^2|$ lead to equations expressed by means of the reverse transfer matrices $\boldsymbol{R}$:

for $x = x_L$ (matrix R_L): (1)

$$\begin{bmatrix} A_L \\ B_L \end{bmatrix} = \frac{m_L}{2\sqrt{k_L \kappa_{1L}}} \begin{bmatrix} \left(\frac{k_L}{m_L} + i\frac{\kappa_{1L}}{m_1} \right) & \left(\frac{k_L}{m_L} - i\frac{\kappa_{1L}}{m_1} \right) \\ \left(\frac{k_L}{m_L} - i\frac{\kappa_{1L}}{m_1} \right) & \left(\frac{k_L}{m_L} + i\frac{\kappa_{1L}}{m_1} \right) \end{bmatrix} \begin{bmatrix} A_1 \\ B_1 \end{bmatrix}$$

for $x = x_1$ to x_{n-1} (matrices R_i): (2)

$$\begin{bmatrix} A_j \\ B_j \end{bmatrix} = \frac{m_j}{2\sqrt{\kappa_{jx_j} \kappa_{(j+1)x_j}}} \begin{bmatrix} \left(\frac{\kappa_{jx_j}}{m_j} + \frac{\kappa_{(j+1)x_j}}{m_{j+1}} \right) e^{S_j} & \left(\frac{\kappa_{jx_j}}{m_j} - \frac{\kappa_{(j+1)x_j}}{m_{j+1}} \right) e^{S_j} \\ \left(\frac{\kappa_{jx_j}}{m_j} - \frac{\kappa_{(j+1)x_j}}{m_{j+1}} \right) e^{-S_j} & \left(\frac{\kappa_{jx_j}}{m_j} + \frac{\kappa_{(j+1)x_j}}{m_{j+1}} \right) e^{-S_j} \end{bmatrix} \begin{bmatrix} A_{j+1} \\ B_{j+1} \end{bmatrix}$$

for $x = x_R$ (matrix R_R): (3)

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = \frac{m_n}{2\sqrt{\kappa_{nR} k_R}} \begin{bmatrix} \left(\frac{\kappa_{nR}}{m_n} - i\frac{k_R}{m_R} \right) e^{S_n} & \left(\frac{\kappa_{nR}}{m_n} + i\frac{k_R}{m_R} \right) e^{S_n} \\ \left(\frac{\kappa_{nR}}{m_n} + i\frac{k_R}{m_R} \right) e^{-S_n} & \left(\frac{\kappa_{nR}}{m_n} - i\frac{k_R}{m_R} \right) e^{-S_n} \end{bmatrix} \begin{bmatrix} A_R \\ B_R \end{bmatrix}$$

where: $k_L = k_L(x_L)$, $k_R = k_R(x_R)$, $\kappa_{1L} = \kappa_1(x_L)$, $\kappa_{nR} = \kappa_n(x_R)$, $\kappa_{jxj} = \kappa_j(x_j)$ and:

$$S_j = \int_{x_{j-1}}^{x_j} \kappa_j dx \tag{4}$$

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

$$A_L \approx R_{1\,1L} \prod_{i=1}^{n-1} R_{1\,1i} R_{1\,1R} A_R \tag{5}$$

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

$$P_{WKB} \approx \frac{\frac{\hbar}{m_R}|A_R|^2}{\frac{\hbar}{m_L}|A_L|^2} = \frac{16\frac{k_L}{m_L}\frac{\kappa_{1L}}{m_1}\frac{\kappa_{nR}}{m_n}\frac{k_R}{m_R}}{\left[\left(\frac{k_L}{m_L}\right)^2 + \left(\frac{\kappa_{1L}}{m_1}\right)^2\right]\left[\left(\frac{\kappa_{nR}}{m_n}\right)^2 + \left(\frac{k_R}{m_R}\right)^2\right]}$$

$$\times \prod_{j=1}^{n-1} \left[\frac{4\frac{\kappa_{jx_j}}{m_j}\frac{\kappa_{(j+1)x_j}}{m_{j+1}}}{\left(\frac{\kappa_{jx_j}}{m_j} + \frac{\kappa_{(j+1)x_j}}{m_{j+1}} \right)^2} \right] \exp\left[-2\int_{x_L}^{x_R} \kappa(x) dx \right] \tag{6}$$

DISCUSSION AND CONCLUSIONS

The term in the product for the j-th interface interior the stack disappears if κ/m is continuous. This proves that the pre-exponential term does not change if the 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 for the simulated structure.

Fig. 3 shows the energy dependence of the tunnelling probability at V_G=1V for three cases of calculations: P_TMM: transfer matrix method, P_exp: only the exponential term of the derived formula (6), P_WKB: full WKB-based formula (6), 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 graph illustrates good accuracy of the WKB based formula for the direct regime of tunneling.

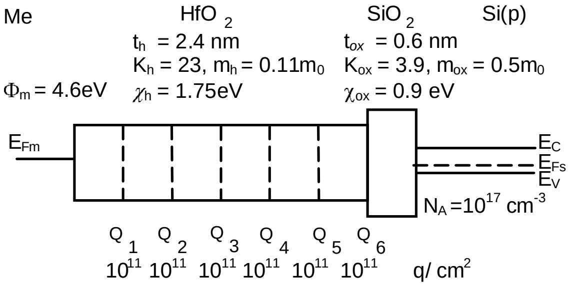

Fig. 2. The simulated gate stack.

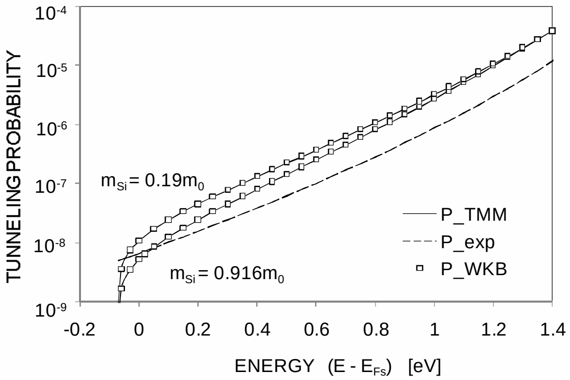

Fig. 3 Energy dependence of the tunneling probability.

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