Modeling Tunneling through Ultra-Thin Gate Oxides

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Charge transport through ultra-thin dielectric barriers is of considerable interest for various applications, such as advanced MOSFETs [1], EPROMs and MIS solar cells. In the thickness range (1-3) nm direct tunneling between the two electrodes of a MOS system is becoming the main mechanism. A fast and accurate computation of the transmission coefficient (TC) $\mathcal{T}(E)$ as function of applied gate voltage is a condition for the numerical simulation of the elastic tunnel current. Restricting to electrons, the current density from the solution of the 1D barrier penetration problem [2] reads:

$$j_n = A_c^* \int_0^\infty d\eta \mathcal{T}(\eta) \ln\left\{\frac{\exp[\eta_{F,S}(d)-\eta_c(d)-\eta]+1}{\exp[\eta_{F,M}(0)-\eta_c(d)-\eta]+1}\right\}$$

with $A_c^* = qm_c^*(k_BT)^2/(2\pi^2\hbar^3)$, $\eta = E/k_BT$, and the normalized quasi Fermi levels $\eta_{F,S}$, $\eta_{F,M}$ of the electrodes. Approximating in-

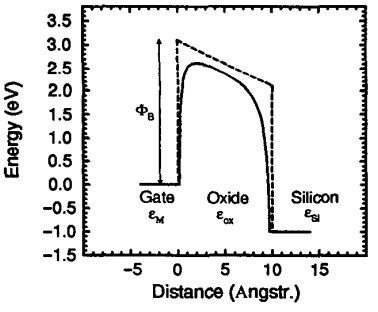

Figure 1: *Idealized potential barrier due to an oxide of 1 nm thickness with (solid curve) and without (dashed curve) image force. Parameters:* $\epsilon_{ox} = 3.9$, $\Phi_B = 3.15\,eV$, $m_{ox} = 0.5\,m_0$.

coming and outgoing states by plane waves, the oxide barrier by a trapezoid (no fixed charges), and assuming a parabolic $E(\vec{k})$ relation in the barrier region as well, the TC is found by the common matching procedure [3]:

$$\mathcal{T}(\eta) = 2\left\{1 + \frac{\pi^2}{2}\left[\frac{m_{Si}k_F}{m_M k_{Si}}\left(\mathrm{Bi}_d'\mathrm{Ai}_0 - \mathrm{Ai}_d'\mathrm{Bi}_0\right)^2 + \right.\right.$$
$$+ \frac{m_M k_{Si}}{m_{Si}k_F}\left(\mathrm{Bi}_d\mathrm{Ai}_0' - \mathrm{Ai}_d\mathrm{Bi}_0'\right)^2 +$$
$$+ \frac{m_M m_{Si}}{\lambda_0^2 m_{ox}^2 k_F k_{Si}}\left(\mathrm{Bi}_d'\mathrm{Ai}_0' - \mathrm{Ai}_d'\mathrm{Bi}_0'\right)^2 +$$
$$\left.\left. + \frac{\lambda_0^2 m_{ox}^2 k_F k_{Si}}{m_M m_{Si}}\left(\mathrm{Bi}_d\mathrm{Ai}_0 - \mathrm{Ai}_d\mathrm{Bi}_0\right)^2\right]\right\}^{-1},$$

where $Ai_0 \equiv Ai\left[\left(\Phi_B - \eta k_BT\right)/\hbar\Theta_{ox}\right]$, $Ai_d \equiv Ai\left[\left(\Phi_B + qF_{ox}d - \eta k_BT\right)/\hbar\Theta_{ox}\right]$ and $\hbar\Theta_{ox} = \left(q^2\hbar^2F_{ox}^2/2m_{ox}\right)^{1/3}$. Φ_B denotes the barrier height for electrons, m_M, m_{ox}, and m_{Si} are the effective electron masses in the three materials, respectively, k_F and k_{Si} are the momenta in the electrodes, and $\lambda_0 = \hbar\Theta_{ox}/qF_{ox}$. The $E_\perp$-dependence of $\mathcal{T}(E)$ was neglected replacing $k_M(E_\perp)$ by the Fermi momentum k_F. The effect of the classical image force on the barrier potential is demonstrated in Fig. 1. Although there is substantial controversy about the image force (the same holds for the value of ϵ_{ox}, the significance of a band structure in case of only a few molecular layers, and the issue of $k_\perp$-conservation), it – or a proper modification – should be most important for ultra-thin oxides with large TCs.

For the purpose of device simulation both the numerical solution of the Schrödinger equation and the WKB approximation, which includes the numerical action integral, are too time-consuming, since the outer numerical integration is unavoidable to obtain the current. An analytical function $\mathcal{T}(E)$ is desirable that takes into account the image force in a better way than by the lowering of a trapezoidal barrier. Based on the observation that the tunnel probability is mainly determined by the action S of the barrier, we propose the following "pseudobarrier method". The actual barrier potential is mapped to a trapezoid (the "pseudobarrier") under the constraint of equal *actions* S:

$$S_{tra}(E) = S_{im}(E)\,,$$

where the subscripts refer to "trapezoid" and "image force". For the thickness d of the

pseudobarrier we use the distance between the two turning points at the energy of the silicon conduction band edge at the interface. The action of the trapezoidal pseudobarrier $S_{tra}(E)$ has a simple analytical form, whereas $S_{im}(E)$ has to be found by numerical integration. In balancing the actions, the barrier height of the trapezoid is released as a free parameter. If this is done for each energy of the tunneling electrons, the barrier height becomes a function of energy. Since $\Phi_B(E)$ results from a numerical iteration, there would be no advantage in terms of CPU time consumption as compared to the WKB approximation. Taking into the bargain some loss in accuracy, we approximate $\Phi_B(E)$ by an analytical function in the following way. The action balance is applied to only three energy values E_j $(j = 0, 1, 2)$ in the lower part of the barrier, which gives us the pseudobarrier heights for these energies. The complete function $\Phi_B(E)$ is then found by parabolic interpolation:

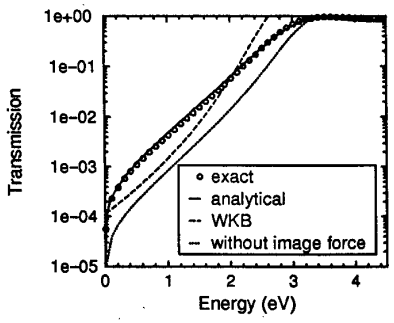

Figure 2: *Calculated transmission probabilities for a MOS structure with 1 nm oxide thickness. Parameters:* $F_{ox} = 10\,MV/cm$, $\epsilon_{ox} = 3.9$, $\Phi_B = 3.15\,eV$, $m_{ox} = 0.5\,m_0$.

$$\Phi_B(E) = \Phi_B(E_0) + \frac{\Phi_B(E_2) - \Phi_B(E_0)}{(E_2 - E_0)(E_1 - E_2)}(E - E_0)(E_1 - E) - \frac{\Phi_B(E_1) - \Phi_B(E_0)}{(E_1 - E_0)(E_1 - E_2)}(E - E_0)(E_2 - E)\,.$$

The accuracy of this approach depends slightly on the choice of $E_{0,1,2}$. However, an excellent overall-agreement with the numerical solution of the Schrödinger equation was found for oxide thicknesses in the range of (0.5-5) nm. Figure 2 illustrates the different approximations in the case of a 1 nm barrier.

The surprising agreement is achieved by varying only one parameter of the pseudobarrier – its height. One and the same set $E_{0,1,2}$ also yields a comparable accuracy for different oxide fields which makes the method applicable to the simulation of IV-curves. Figure 3 was obtained assuming that $E_c(d) - E_{F,S}(d) = 0.2\,eV = const$ and that the voltage drops only over the barrier. In Fig. 4 the voltage range was extended to the Fowler-Nordheim regime. Again, the pseudobarrier method gives results very close to the numerical solution of the Schrödinger equation.

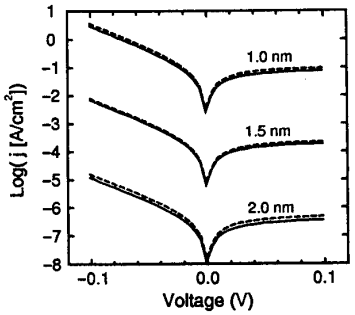

Figure 3: *IV-characteristics of an Al-SiO_2-Si(n) diode for different oxide thicknesses. Solid curves: numerical solution of the Schrödinger equation, dashed curves: pseudobarrier method. Parameters:* $\epsilon_{ox} = 2.13$, $\Phi_B = 3.15\,eV$, $m_{ox} = 0.5\,m_0$.

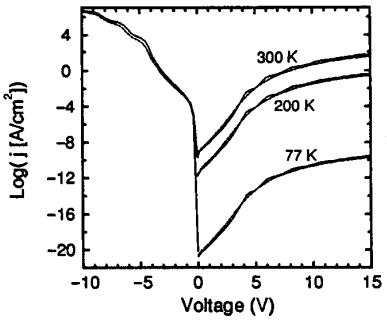

Figure 4: *IV-characteristics of an Al-SiO_2-Si(n) diode with 2.5 nm oxide thickness for different temperatures. Solid curves: numerical solution of the Schrödinger equation, dashed curves: pseudobarrier method. Parameters: see Fig. 3.*

References

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[2] P. J. Price and J. M. Radcliffe. Esaki Tunneling. *IBM Journal*, Oct.:364–371, 1959.

[3] K. H. Gundlach. Zur Berechnung des Tunnelstroms durch eine trapezförmige Potentialstufe. *Solid-State Electronics*, 9:949–57, 1966.