The Role of Quantization Effects in Inversion Hole Layers of Tunnel MOS Structures on n-Si Substrates

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Abstract

Disregarding the quantum effects in inversion hole layers was shown to result in the false calculation of the distribution of the applied voltage in a tunnel MOS structure which consequently provokes substantial errors in estimating the tunnel currents and the energy of injected electrons.

1. Introduction

Recent experimental studies of the reliability of ultrathin SiO_2 films (see, e.g., [1]) in the direct-tunneling mode have clearly demonstrated, that the application of tunnel oxides as gate dielectric in MOSFETs [2], as well as in transistors [3,4] and thyristors [5] with a tunnel MOS emitter, looks quite realistic. Therefore the demand on the accurate modeling of a tunnel MOS structure becomes evident, and earlier half-quantitative analyses cannot be longer considered satisfactory.

An important step toward formulating an exact description of this structure is, in our opinion, the inclusion of quantization of hole motion in the inversion layer into the model. In this paper we first perform a complete quantum treatment of a tunnel MOS structure under reverse bias ("+" to n-Si), which is the normal operation condition for most tunnel MOS devices [2-5]. To be specific, we concentrate on the bipolar $Al/SiO_2/n$-Si tunnel MOS emitter transistor with an induced base (Fig.1). The results are compared with those obtained within the previously developed "classical" models.

2. Calculations of the band diagram and tunnel currents

An exact treatment for an inversion layer in the tunnel MOS structure presumes the self-consistent solution of the Poisson and Schrödinger equations:

$$-\frac{\hbar^2}{2m_{i,z}}\frac{d^2\psi_{i,j}}{dz^2}+q\varphi\psi_{i,j}=\left(E_{i,j}-\left[\begin{array}{l}0\,,\ \text{for } i=hh,lh\\ \Delta E_{so}\,,\ \text{for } i=so\end{array}\right.\right)\psi_{i,j} \qquad (1)$$

$$\frac{d^2\varphi}{dz^2}=-\frac{q}{\varepsilon_0\varepsilon_s}\left(N_D+\sum_i\sum_{j=0}^{j_{max}(i)}N_{i,j}\left|\psi_{i,j}\right|^2\right) \qquad (2)$$

like it is usually done in MOSFETs [6,7], with boundary conditions for the wave functions: $\psi_{i,j}|_{z=0,+\infty} = 0$. N_D is the donor concentration, ε_s is the permittivity of the semiconductor, ΔE_{so} is the energy of the spin-orbital splitting and $m_{i,z}$ is the hole effective mass in the z-direction (orthogonal to the Si/SiO_2 interface plane). The solution of (1,2) yields the values of energy levels for holes $E_{i,j}$ and their occupancies $N_{i,j}$ ($j = 0, 1, \ldots, \infty$). The subscript i means "heavy holes"(hh), "light holes"(lh) or "holes in the spin-splitted-off subband"(so). Simultaneously, the Fermi energy for holes E_{Fp_s} (see also Fig.2) may be found from

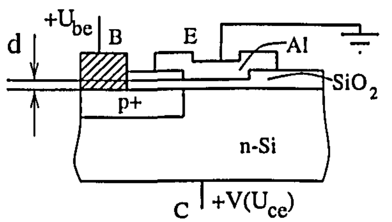
$$N_s = \sum_{i,j} N_{i,j} = kT \sum_i \frac{m_{i,\perp}}{\pi \hbar^2} \sum_{j=0}^{j_{max}(i)} \ln\left(1 + \exp\left(\frac{E_{Fp} - E_{i,j}}{kT}\right)\right) \tag{3}$$

where N_s is a two-dimensional (2D) hole density in the inversion layer, $m_{i,\perp}$ is the transverse hole mass in the i-th subbands and T is a temperature. Having the coordinate dependence of a potential $\varphi(z)$ obtained, the valence (conduction) band profile $E_{v(c)}(z) = E_{v(c)0} - q\varphi(z)$ will be automatically determined.

An expression for the hole tunnel current should be written as a sum of currents from the discrete levels, instead of a "classical" integral over the hole energy [3], namely

$$j_h = q \sum_{i,j} N_{i,j} \frac{qF_s}{2\sqrt{2m_{i,z}}} E_{i,j}^{-1/2} \Theta_h(E_{i,j}) \sim q \sum_{i,j} N_{i,j} \frac{E_{i,j}}{h} \Theta_h(E_{i,j}) \tag{4}$$

where Θ_h is a tunneling probability and F_s is the electric field in silicon just near the Si/SiO_2 interface. The hole leakage was shown to affect the subband structure very weakly (a shift of the ground energy level $\Delta E/E_{hh,0}$ is less than 10^{-8} for a 2.0-nm oxide), so that the "separate" calculation of the band diagram (as if there were no charge transport) followed by a computation of the tunnel currents is justified.



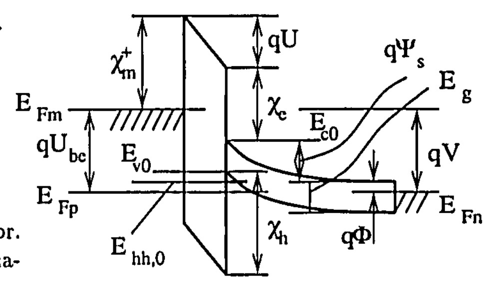


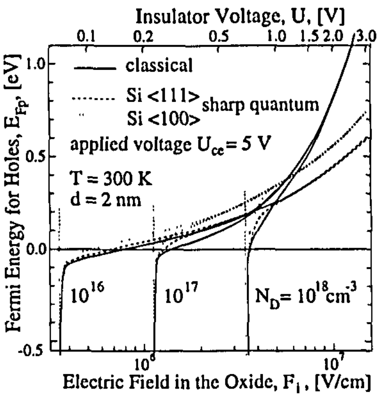
Fig.1. Tunnel MOS emitter transistor.
Fig.2. (right) The energy band diagram with a notation used in text.

The tunnel parameters used for the calcluations are $\chi_e = 3.15$eV, $\chi_m^+ = 3.17$eV (Fig.2), oxide thickness $d = 2.0$nm. An effective mass of tunneling electrons in SiO_2 was taken $m_e^I = 0.30m_0$. The so-called one-band model of insulator was adopted [3], which uses $\chi_h = \chi_e + E_g = (3.15 + 1.12) = 4.27$eV, and the tunneling hole mass $m_h^I = m_e^I$. Si substrate orientation was (100) or (111). The hole masses in the inversion layer $m_{hh,z}^{100} = 0.291m_0$, $m_{hh,\perp}^{100} = 0.433m_0$, $m_{lh,z}^{100} = 0.200m_0$, $m_{lh,\perp}^{100} = 0.169m_0$, $m_{hh,z}^{111} = 0.746m_0$, $m_{hh,\perp}^{111} = 0.549m_0$, $m_{lh,z}^{111} = 0.141m_0$, $m_{lh,\perp}^{111} = 0.151m_0$ were taken. The spin-splitted subband (ΔE_{so} =0.044eV) was characterised by the isotropic mass $m_{so} = 0.290m_0$. The effective density-of-state mass for electrons in the interface plane was assumed to be $m_{e,\perp}^{111} = 2.2m_0$. The "classical" solution (for reference) was performed in the spirit of an earlier work [3].

3. Quantization-related effects in a tunnel MOS structure

In addition to the 2D effects observable in MOSFETs (non-trivial behaviour of a low-temperature conductivity of the inversion layer etc. [6,7]), quantum phenomena are expected to be revealed in the currents flowing in the tunnel MOS structure.

Figs.3-6 represent the dependencies of the Fermi energy ($E_{Fp} > 0$, if the interface is degenerated) on F_i, valence band profile $E_v(z)$ in Si, as well as tunnel currents j_e and j_h. The discrepancies between the classical and quantum results are evident.



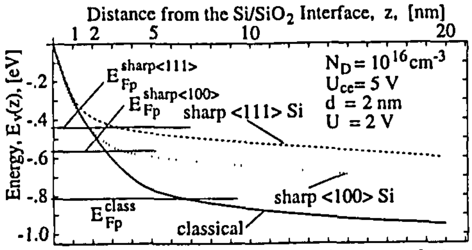


Fig.3. (left) The dependencies of the Fermi energy for holes E_{Fp} on the electric field in the insulator.

Fig.4. The profile of the valence band $E_v(z)$. The surface potential Ψ_s is 2.814 V for all curves.

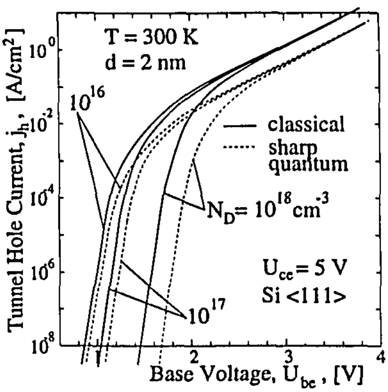


Fig.5. The hole tunnel current j_h vs. the base voltage.

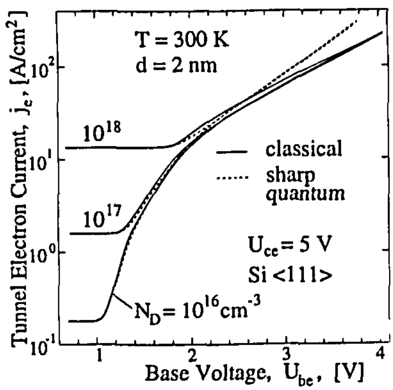


Fig.6. The electron tunnel current j_e (calculated like in [3]).

Incorrect classical estimation of E_{Fp} leads to the prediction of a false interrelation between the measured terminal voltage U_{be} and the insulator bias $U = U_{be} - (E_g + E_{Fp} + \chi_e - \chi_m^+)/q$. An error in E_{Fp} introduced by a classical treatment (Fig.3) should be considered large, since the tunnel currents depend on U very strongly.

The knowledge of the conduction band profile (Fig.4) is essential for studying the energy relaxation of injected hot electrons (impact ionization [4], light emission). Even a small error in $E_v(z)$ is intolerable, in particular because the quantum yield of ionization $P(E_e)$ increases unusually rapidly (more rapidly than $\sim 10^3$ times/eV) in the corresponding range of electron energies E_e.

Taking the ionization into account, the collector current j_c is equal to $j_e + j_e \cdot P$ and the base current j_b - to $j_h - j_e \cdot P$ [4]. Calculations show that the "classical" values of a current gain $\beta = j_c/j_b$ are lower than the true ones. For $U_{be} \sim 2$V or less (i.e. while P=0), it is also clear from the inspection of Figs.5,6.

4. Conclusion

In this paper we have demonstrated that the classical treatment of an inversion layer in the tunnel MOS structure leads to the following errors:
(i) The interrelation between measured base and collector voltages (U_{be}, U_{ce}) and insulator bias U, is predicted incorrectly, it results in the incorrect evaluation of currents.
(ii) A difference between (100) and (111) substrates is almost completely ignored.
(iii) The classically calculated profile of the valence band in silicon differs from the exact one considerably.
(iv) The current gain of a tunnel MOS emitter transistor is substantially underestimated.
In common, we may conclude that the 2D-consideration of the hole gas in the inversion layer is essential for a correct modeling of the tunnel MOS structure on (100) n-Si and (111) n-Si substrates. The quantization effects are shown to be important almost in all practically interesting operational modes [2-5], especially for high insulator bias and high doping concentration N_D.

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References

[1] M. Depas, B. Vermeire, P.W. Mertens, M. Meuris and M.M. Heyns, "Wear-out of ultra-thin gate oxides during high-field electron tunneling," *Semicond. Sci. Technol.*, vol. 10, pp. 753-758, 1995.

[2] H.S. Momose, M. Ono, T. Yoshitomi, T. Ohguro, A. Nakamura, M. Saito and H. Iwai, "1.5 nm direct-tunneling gate oxide Si MOSFETs," *IEEE Trans. Electron Devices*, vol. ED-43, no. 8, pp. 1233-1242, 1996.

[3] K.M. Chu and D.L. Pulfrey, "An analysis of the DC and small-signal AC performance of the tunnel emitter transistor," *IEEE Trans. Electron Devices*, vol. ED-35, no. 2, pp. 188-194, 1988.

[4] I.V. Grekhov, A.F. Shulekin and M.I. Vexler, "Silicon Auger transistor - new insight into the performance of a tunnel MIS emitter transistor", *Solid-State Electron.*, vol. 38, no. 8, pp. 1533-1541, 1995.

[5] W.K. Choi and A.E. Owen, "A thyristor model of switching in metal-thin insulator-semiconductor-semiconductor devices: the influence of insulating layer and illumination,", *J. Appl. Phys.*, vol. 68, no. 12, pp. 6447-6452, 1990.

[6] T. Ando, A.B. Fowler and F. Stern, "Electronic properties of two-dimensional systems", *Rev. Mod. Phys.*, vol. 54, no. 2, 1982.

[7] C.-Y. Hu, S. Banerjee, K. Sandra and R. Sivan, "Quantization effects in inversion layer of PMOSFET's on Si(100) substrates", *IEEE Electron Device Letters*, vol.17, no. 6, pp. 276-278, 1996.