Nuclear Modeling of Quantum Gate Leakage Currents with Sensitivity Analysis

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***Abstract** - A new formulation for gate-leakage currents due to quantum tunneling is presented. The resulting model has been inserted into software modules. The relative importance of various gate stack design parameters is investigated using DOE/RSM methods.*

INTRODUCTION

With the downscaling of deep sub-micron CMOS, the corresponding downscaling of the insulating dielectric has become a major design concern. Device integration into full circuits demands that gate-voltage swings be com-parable to source-drain voltage swings. This has forced the thickness of oxides into the nanometer region. Ultra-thin oxides suffer from low reliability. Therefore, alternative dielectrics such as Ta_2O_5, ZrO_2 and mixtures of SiO_2 with Si_3N_4 are investigated. Many of these oxides have rather low barrier heights such that despite their high-k values and thick size (5 nm) the quantum leakage currents must be considered. For this purpose we have developed a theory for quantum tunneling currents that is capable of handling an arbitrary stack of insulating materials (potential-barrier steps). By treating the full system of the substrate, the inversion layer, the gate stack and the gate metal as a single quantum-mechanical many-electron sys-tem in a Fang-Howard like approximation [1], the subband states appear as resonances in the probability for finding the electrons in some subband state. These resonances can be described using the formalism of Breit and Wigner [2] that was developed as a theory for nuclear decay. Contrary to nuclear states that decay only once (per nucleus), the subband states may be refilled and contribute to the gate current again.

THEORETICAL RESULTS

The key result of the Breit-Wigner approach to subband decay is that the current density at instant t>0, arising from the subband state $|\alpha l k\rangle$ being occupied at t=0, is

$$J^{z}_{\alpha l \vec{k}}(\vec{r},z,t)=\frac{1}{L_x L_y}\frac{e}{\tau_{\alpha l}}e^{-2(\mathrm{Im}(k_z)(z+T_{ox})+\Gamma_{\alpha l}t/\hbar)}$$

where $\tau_{\alpha l}=\hbar/4\pi\Gamma_{\alpha l}$ relates the lifetime of the eigenstate $|\alpha l k\rangle$ to the resonance width. Assuming instantaneous refilling of the sub-bands after decay and summing all subband contributions to the gate current by an assemble average under biased conditions, the gate current becomes and $W_{\alpha l}$ represents the real part of the complex energy eigenvalue $W= W_{\alpha l}+i\Gamma_{\alpha l}$. The core of the calculation of the gate current deals with the evaluation of the subband

$$J_G=-\frac{ekT}{\pi\hbar^2}\sum_{\alpha l}\frac{\sqrt{m_{\alpha x}m_{\alpha y}}}{\tau_{\alpha l}}\times$$
$$\log\frac{1+\exp(E_F-W_{\alpha l}-eV_G)/kT}{1+\exp(E_F-W_{\alpha l})/kT}$$

lifetimes. For this purpose we exploited a trans-fer matrix method to incorporate the arbitrary stack of insulating layers and by using the fact that subband resonances appear as resonances of Lorentz shapes in the probability $P_\alpha(W)$ of finding a carrier in some energy W (Fig. 1):

$$P_\alpha(W)\rightarrow\sum P_\alpha(W_{\alpha l})\frac{\Gamma^2_{\alpha l}}{(W-W_{\alpha l})^2+\Gamma^2_{\alpha l}}$$

$$\text{and }\Gamma^2_{\alpha l}=2P^{-1}_\alpha(W_{\alpha l})\left[\frac{\partial^2 P^{-1}_\alpha}{\partial W^2}(W_{\alpha l})\right]^{-1}.$$

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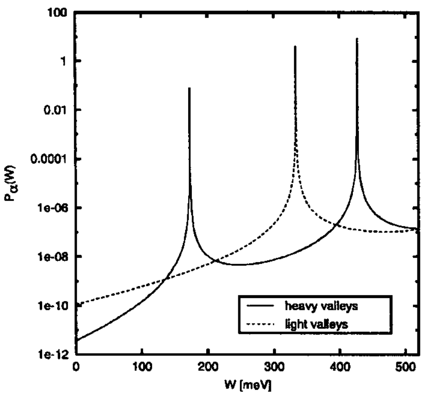

Fig.1 Resonances in the probability for finding an electron in the gate region with energy W.

SOFTWARE MODULES AND SENSITIVITY

We have developed a code (SCALPEL) that evaluates gate leakage currents according to above ideas. The gate leakage currents of inversely biased MOS capacitances was calculated and compared with experimental data. As an example, in Fig.2 the simulated and experimental curves for a 2.5-nm oxide are shown.

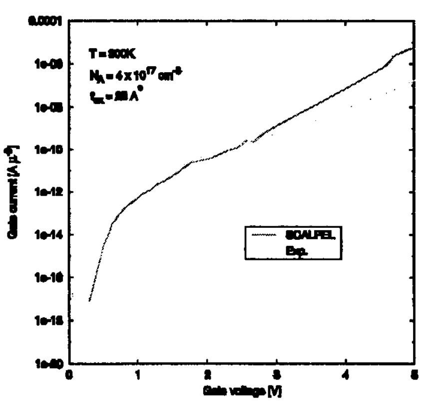

Fig.2 Gate tunneling current for NO layer of 2.5 nm and substrate doping of $4x10^{17}$ cm^{-3}.

We have performed a sensitivity analysis for the engineering of gate stacks using a DOE-RSM approach, using the logarithm of the leakage current as response and layer thickness, the effective masses in the insulating material, the permittivities and the barrier heights as design parameters, i.e. material engineering.

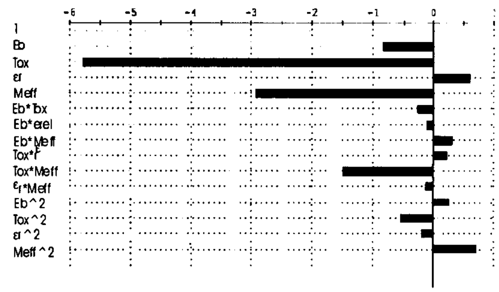

Fig.3 Ranking of model terms in rsm using a CCF design of experiment.

Fig.3 shows the relative contribution of the various design parameters to the leakage current. Plotting actual simulation data vs. response-surface model data (Fig 4) inspects the quality of the response surfaces. Good models are obtained by 2nd order polynomials. The sensitivity analysis demonstrates that the effective mass of the carriers in the insulating stack is a top-two contributor for suppressing gate leakage currents.

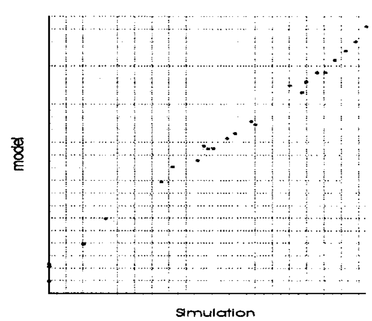

Fig.4 Quality plot of the 2nd order polynomial design. T_{ox} and m_{eff} are the top-2 parameters.

CONCLUSION

A new model for quantum leakage currents is presented. The model is used for finding the critical design parameters for controlling gate leakage.

REFERENCES

[1] F.F. Fang and W.E. Howard, Phys. Rev. Lett. **16**, 797 (1966)

[2] G. Breit and E.P. Wigner, Phys. Rev. **49**, 519 (1936)