Extended Abstracts of the 2001 International Conference on Solid State Devices and Materials, Tokyo, 2001, pp. 140–141

F-1-4

Quantum Mechanical Analysis of Accumulation Layers in MOS Structures

Shin-ichi Saito and Kazuyoshi Torii

Hitachi, Ltd., Central Research Laboratory
1-280, Higashi-koigakubo Kokubunji-shi, Tokyo 185-8601, Japan
Phone:+81-42-323-1111 Fax:+81-42-327-7773 E-mail:Shinichi-crl.Saito@c-net3.crl.hitachi.co.jp

1. Introduction

Many high-k materials have recently been investigated as an alternative gate dielectric for sub-100-nm MOSFETs. Equivalent oxide thickness (EOT) is a primary criterion for assessing candidates. However, there exists up to 20% difference in EOT values extracted from capacitance-voltage (CV) characteristics depending on simulation packages [1]. The fully self-consistent numerical simulation [2] has been developed but it takes a long time to calculate CV curves. On the other hand, to our knowledge, the analytical solution for accumulation conditions has not been obtained, because the problem is intrinsically quite complicated. In this paper, we propose a simple new analytical model based on the *exact* solution of an *exponential potential* to quantify CV curves in accumulation conditions, within a practical calculation time.

2. Theory

We have analyzed the potential $\phi(z)$ by the Fang-Howard wave function [3], and found $\phi(z)$ depends exponentially on the distance from interface, z. Accordingly, we assume $\phi(z)$ as

$$\phi(z) = \phi_s e^{-\frac{z}{W}}, \quad (1)$$

which satisfies the boundary conditions, $\phi(0)=\phi_s$ and $\phi(\infty)=0$. Width W of $\phi(z)$ is determined by Gauss' law as a function of total accumulation charge Q_{tot}. Using this potential, we can solve Schrödinger eq. exactly and thus get the wave function represented by the Bessel function J as

$$\Psi_{ij}(z) = J_{2\tilde{k}_{ij}W}\left(2k_j W e^{-\frac{z}{W}}\right), \quad (2)$$

where i (j) is the subband (valley) index, and k_j is defined as $\sqrt{2m_j e|\phi_s|}/\hbar$ and $\tilde{k}_{ij}$ as $\sqrt{2m_j|E_{ij}|}/\hbar$. Here, $\Psi_{ij}(z)$ satisfies the boundary conditions, $\Psi_{ij}(\infty)=0$ and $\Psi_{ij}(0)=0$, and the latter gives the quantized energy level $E_{ij} = -|E_{ij}| <0$. We have taken all energy levels into account in calculating Q_{tot}, and obtained the self-consistency condition for Q_{tot} by quantum statistics. Solving for Q_{tot} at each ϕ_s gives us CV curves. Although this solution is consistent with Schrödinger eq., quantum statistics, and Gauss' law, Poisson eq. is not satisfied exactly at each point z. The accuracy of our assumption was confirmed by solving Poisson eq. with charge distribution given by eq. (2). As shown in Fig.1, the difference between initial $\phi(z)$ and obtained one is less than 1%. The potential obtained by classical model is logarithmic and this significant difference makes it difficult to converge numerical simulations that initiate from classical potential.

3. Results and Discussions

The calculated CV curve is in good agreement with measured data without any fitting parameters (Fig. 2). Capacitance C_{tot} determined by quantum mechanical analysis is less than that determined by classical models based on either Fermi-Dirac (FD) or Maxwell-Boltzmann (MB) statistics. The difference originates from the formation of the "accumulation layer" away from the interface, as shown in Fig. 3. In Fig. 4, we have conformed that our exponential potential model is consistent with numerical simulations of Ref. [2], however, the linear (triangular) potential model [3] fails to match these results. Since our method is based on an analytical model, it takes only a few minutes to calculate a CV curve by PC. As shown in Fig. 5, substrate component of the capacitive effective thickness CET (t_{Si}) remains finite at V_g=-3.0 V. Thus, quantum effects cannot be neglected even at high electric fields. The difference of CET between quantum-mechanically calculated CET (CET_{QM}) and classically calculated CET (CET_{FD}) is shown in Fig. 6. As EOT becomes thinner, the quantum mechanical correction increases, and it exceeds 20% at EOT=1.0 nm. The difference between EOT extracted by the present model and optical thickness is within 1 Å for both NMOS and PMOS (Fig. 7). Figure 8 shows the dependence of EOT on CET. EOT values can easily be estimated from the measured CV data by the formulas in the insets of Fig. 8.

4. Conclusions

We propose a simple analytical model to quantify CV curves. The accumulation potential turns out to be well approximated by exponential rather than linear or logarithmic. Using exponential potential, Schrödinger eq. is exactly solved consistent with quantum statistics and Gauss' law. The determination of ultra-thin oxide thickness is possible based on an excellent agreement between measured and modeled CV curves.

Acknowledgments

We would like to thank H. Miki, T. Onai, D. Hisamoto, R. Tsuchiya, K. Ohnishi, T. Yamauchi, S. Tsujikawa, K. Watanabe, M. Ogasawara, M. Hiratani, and S. Kimura for their useful discussions and experimental data.

References

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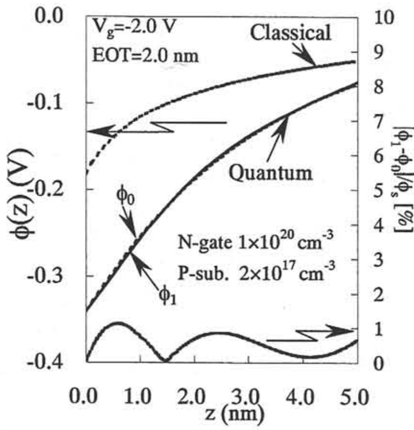

Fig. 1 Exponential potential ϕ_0, iterated potential ϕ_1, and classical potential. The difference is also shown.

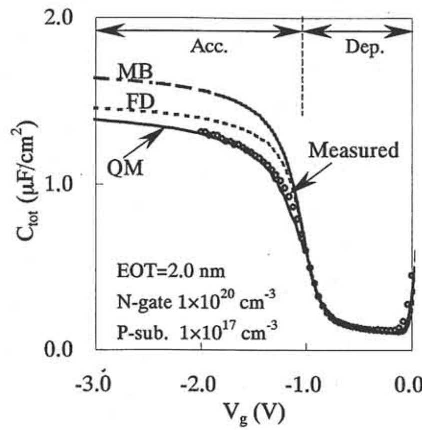

Fig. 2 Total gate capacitance C_{tot}, calculated by quantum mechanical model (QM), classical model, and measured C_{tot}.

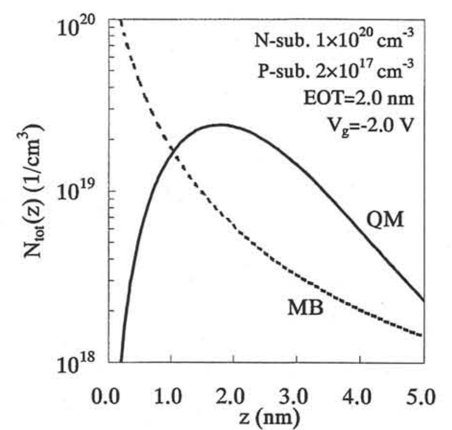

Fig. 3 Charge distribution $N_{tot}(z)$ calculated by our quantum mechanical model (QM) and classical model (MB).

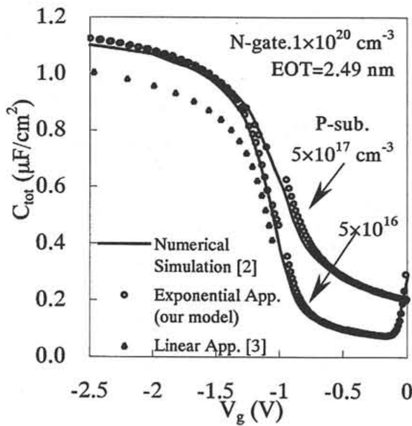

Fig. 4 Comparison of exponential approximation with numerical simulations [2] and linear approximation [3].

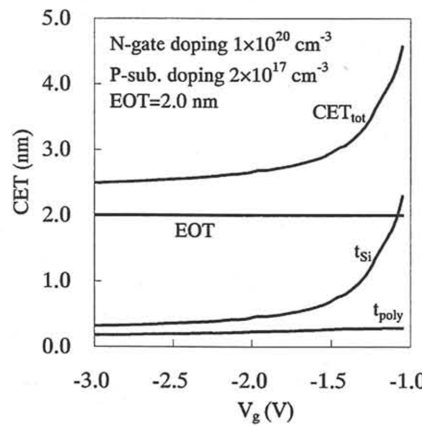

Fig. 5 Dependence of CET ($= \varepsilon_{SiO2}/C$) on V_g. CET for total, substrate, and poly-Si gate capacitance is CET_{tot}, t_{Si}, and t_{poly}.

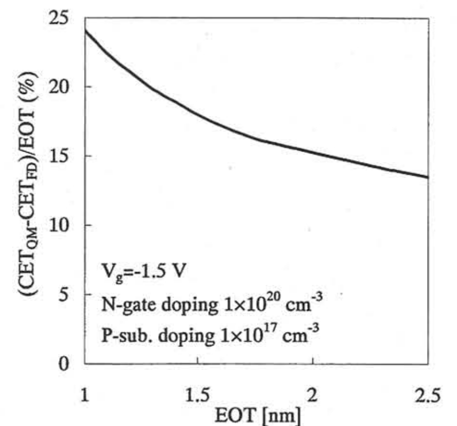

Fig. 6 Difference between CET_{QM} and CET_{FD}. Quantum corrections become more important as EOT decreases.

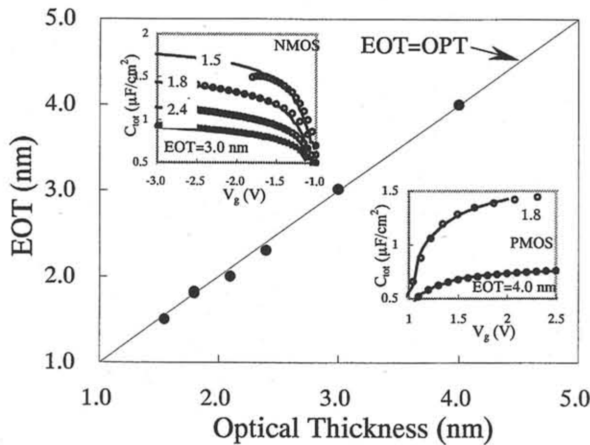

Fig. 7 Comparison between optically measured oxide thickness (OPT) and EOT extracted from CV curves.

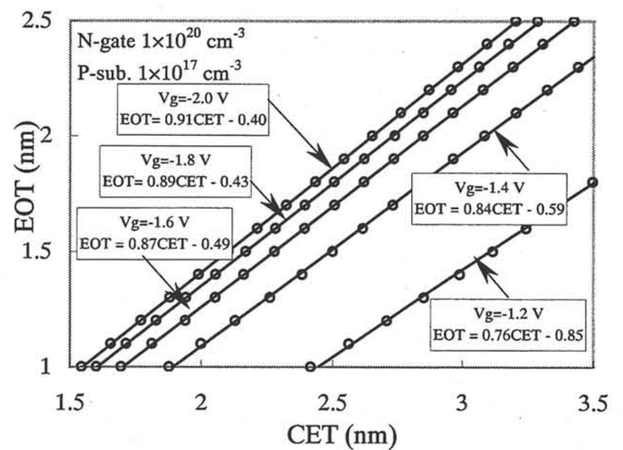

Fig. 8 EOT dependence of CET. Formulas are shown in the insets corresponding to various V_g.