# Density-Gradient Simulations of Quantum Effects in Ultra-Thin-Oxide MOS Structures

M.G. Ancona
Naval Research Laboratory
Washington, DC 20375
ancona@sinh.nrl.navy.mil

Z. Yu, W.-C. Lee and R.W. Dutton
Center for Integrated Systems, Stanford University
Stanford, CA 94305

P.V. Voorde
ULSI Laboratory, Hewlett-Packard
Palo Alto, CA 94306

Abstract--The density-gradient approach to quantum transport theory is used to model the C-V characteristics of MOS devices with ultra-thin gate oxides. The method is shown to provide a physics-based approach the works well in all bias regimes and is simple enough for engineering applications.

## I. INTRODUCTION

The current generation of metal-oxide-semiconductor (MOS) devices have oxide thicknesses of roughly 80Å and it is expected that, with further device scaling deeper into the submicron regime, oxides in the thickness range of 20-50Å will become of great technological importance [1]. To understand the characteristics of these devices it becomes increasingly important to take effects of quantum mechanics into account. The most obvious quantum mechanical effect, seen in the very thinnest oxides, is gate leakage via direct tunneling through the oxide. The exponential turn-on of this effect sets the minimum practical oxide thickness (~20Å). Above this thickness, tunneling is insignificant but a second effect, the quantum mechanical repulsion of electrons/holes from the vicinity of the Si-$SiO_2$ interface, can still be quite important. In particular, this repulsion will impact the electrical characteristics when the distance over which it is felt (typically ~5Å) is a non-negligible fraction of the oxide thickness. The purpose of the present work is to model this exclusion effect using an approximate quantum treatment known as density-gradient theory [2]. We focus on interpreting C-V data since this is an essential tool for characterizing critical device parameters such as threshold voltage, gate capacitance and doping profiles [3].

Efforts to understand the effects of quantum mechanical repulsion and confinement in inversion layers date back to the pioneering work of Stern and co-workers [4]. More recently, with the recognition that such effects become important technologically as oxide thickesses are reduced, a number of additional theoretical studies have been undertaken including "exact" Poisson-Schrodinger calculations [5] and various classical simulations with *ad hoc* quantum corrections [6,7]. In principle, the Poisson-Schrodinger approach is the best since it fully includes the quantum mechanics (in a one-electron framework). However, it is not well-suited to engineering application and it is not easily generalized (e.g., to greater than one-dimension or to non-equilibrium situations) though a number of efforts attempting to do so have appeared [8]. In contrast, the phenomenological approaches are typically within a continuum framework, e.g., diffusion-drift, and are therefore easy to apply. Unfortunately, they suffer from not having a solid physical foundation and hence are able to match measured data only in limited regimes and then only by curve-fitting. They do not have much predictive or extrapolative value and their parameters do not have well-defined

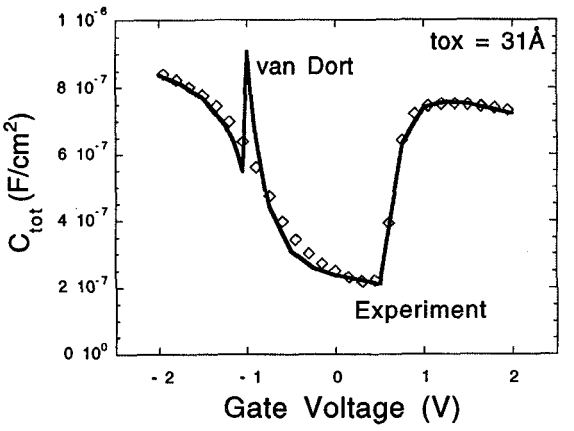


Fig. 1. Comparison of the experimental C-V curve (diamonds) with the best fit using the method of van Dort [6] (solid line). The poly doping is taken to be 4 x $10^{19}$cm$^{-3}$.

physical meanings. As an example, in Fig. 1 we plot the best fit of the model of van Dort [6] together with some experimental data for an MOS capacitor with a 31Å gate oxide.

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This model, which merely corrects the band edge with a fitting parameter, does capture the basic characteristic but it is obviously reasonable only in a restricted range. A similar comparison for the model due to Hansch [7] is shown in Fig. 2. The Hansch model's derivation [7] suggests a more solid physical basis than the van Dort model, however, as shown in the Figure when the electron wavelength in the model is given its correct thermal value (12Å), the simulation results are rather poor. Only by using an unphysically large electron wavelength (40Å) do reasonable fits to data become possible (see Fig. 2). But note that even in this case, the fit has the wrong slope in strong accumulation (large negative voltage for this p-type sample), a regime where quantum effects dominate, errors in the doping profiles play no role and one would expect the model to do best. Another problem is an unphysical change in slope observed at flatband. And of course, like the van Dort model, the Hansch model (with the electron wavelength used as a curve-fitting parameter) provides little understanding of the sources of these various discrepancies. As an alternative continuum approach, in this paper we explore the use of density-gradient theory for performing such simulations. This theory is physically well-founded yet is simple enough to be useful in engineering-oriented applications. As we show, it can allow the C-V behavior in all regions of operation to be modeled and understood.

## II. DENSITY-GRADIENT THEORY

Density-gradient theory is an approximate quantum transport theory which can be derived using methods of continuum field theory or directly from quantum mechanics [2]. In macroscopic terms it captures the non-locality of quantum mechanics to lowest-order by assuming the electron gas is energetically sensitive to both the density and the gradient of density. This assumption gives rise to equations of state for the electrons and holes as sums of classical density-dependent terms plus quantum terms that are density-gradient-dependent. Written in chemical potential form the equation of state for the electron gas at lowest order can be shown to be [2]

$$\varphi^e_{DG} = \varphi^e_{DD}(n) + 2b\frac{\nabla^2\sqrt{n}}{\sqrt{n}} \qquad (2.1)$$

where n is the electron density and $\varphi^e_{DD}$ is the classical (diffusion-drift) chemical potential which we assume to take a Fermi-Dirac form [9]. The quantity b is the (linear) density-gradient coefficient which gauges the strength of the gradient effect in the gas. The choice of the value for this coefficient is crucial and in this work we take it to have the theoretical "high" temperature value of $b = \hbar^2/(12m^*q)$ [10] where $m^*$ is an effective mass whose value is discussed below. Inserting this into the equation of momentum balance (assuming inertia negligible [11]) gives

$$\vec{J}_n = n\mu_n\nabla\varphi - D_n\nabla n + 2nb\mu_n\nabla\left(\frac{\nabla^2\sqrt{n}}{\sqrt{n}}\right) \qquad (2.2)$$

where

$$D_n = n\mu_n\frac{\partial\varphi^e_{DD}}{\partial n}$$

and all other quantities have their usual meanings. When the gradient of n is small the third term of the current equation is negligible and the electron gas behavior is governed by the standard diffusion-drift current equation. However, when steep gradients are encountered (as in accumulation/inversion layers)

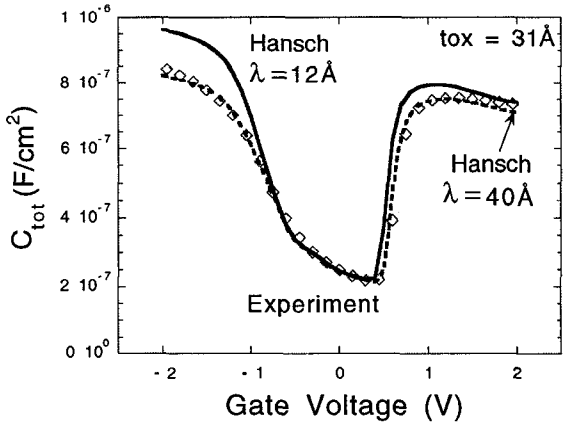


Fig. 2. Comparison of the experimental C-V curve (diamonds) with that computed using the method of Hansch [7] assuming the correct electron wavelength (solid line) and using it as a curve-fitting parameter (dashed line).

the third term becomes non-negligible and "quantum" behavior is manifested, e.g., (2.2) will describe tunneling phenomena [11]. The theory is completed with the addition of similar equation for holes, charge balance equations for electrons and holes, the Poisson equation of electrostatics and a set of consistent boundary conditions. The complete theory has been applied to a variety of situations in both semiconductors [2,11-13] and metals [10] and appears to be quite useful.

The application of these equations to the MOS inversion layer was in fact their original application [2] and all of the analysis and discussion of the earlier work is relevant here. The primary new aspect of the present work is the testing against experimental data. Also new here is the application to all bias regimes (which requires consideration of both carrier types) and the treatment of a non-ideal gate. To analyze the MOS situation we set up and solve a one-dimensional boundary value problem which includes the equilibrium (zero current) form of (2.2), an analogous equation for holes, an electrostatic equation which includes incomplete ionization of impurities and a non-ideal polysilicon gate. The doping profiles in the Si substrate have been measured with SIMS [3] and that in the polysilicon gate is assumed constant with its value being obtained by fitting the C-V curve in strong inversion. To solve these equations requires numerical methods and, for this purpose, we have found a Newton iteration to be quite robust and efficient. (Our earlier work employed a

shooting method iteration which was efficient but occasionally unstable). A small-signal ac analysis, solved in one pass of the linear system solver, is used to find the differential capacitance.

## III. RESULTS

As computed using density-gradient theory, the effects of quantum mechanics on the carrier profiles in a poly-gate capacitor biased in inversion are shown in Fig. 3. The main consequence is the exclusion of carriers from the oxide which causes their densities to fall to zero at the oxide interfaces. Note that the near-interface drop in the electron density in the

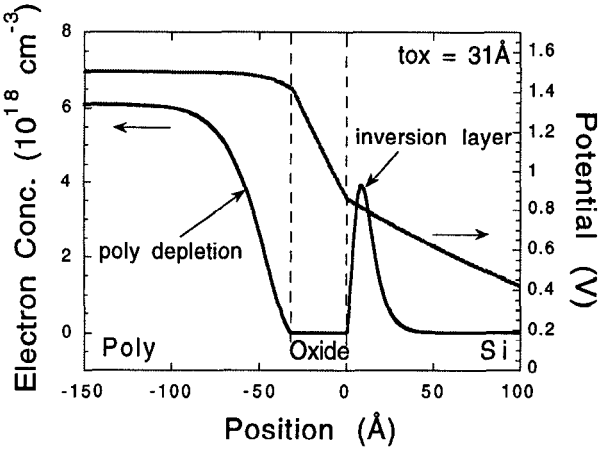


Fig. 3. Electron concentration and potential profiles in inversion (V=1.5) as computed using density-gradient theory.

relatively low doped n-type poly-gate is largely the result of classical depletion (though right at the poly-oxide interface quantum exclusion does occur). Qualitatively, these are the expected results. We attempt no quantitative comparison of these profiles with Poisson-Schrodinger predictions because a number of such comparisons (for much simpler situations) have already been carried out [2]. In general, these previous studies demonstrate density-gradient theory to be quite accurate even at rather small spatial scales; its only qualitative failure is an inability to describe interference phenomena which, for example, give rise to Friedel oscillations in the density when the well is very shallow.

The effect of the quantum mechanical profiles on the C-V characteristics are studied next. In Fig. 4, we plot C-V curves computed classically (diffusion-drift) and using density-gradient theory and compare them with experimental data for the same sample as in Figs. 1 and 2. For both calculations there are *no* fitting parameters apart form the assumed-uniform poly doping ($2.4 \times 10^{19}$cm$^{-3}$). The evident failure of the classical calculation shows the importance of the quantum effects. As seen from the Figure, including these effects in the density-gradient approximation greatly improves the agreement especially in accumulation. For this calculation the effective masses normal to the surface (used as m* in (2.2)) have been assumed to take their largest values (longitudinal electron mass and heavy hole) to reflect the fact that the heavy carriers approach the interface most closely and therefore dominate the capacitance. In inversion the agreement is less good; this is not believed to be caused by errors in the treatment of the quantum effects but rather is probably due to uncertainties in the poly doping profile and resultant inaccuracies in the poly depletion. In any event, density-gradient theory clearly provides continuous and smooth results for all gate voltages unlike the other methods. It is especially meaningful that it works best in strong accumulation where doping effects (in the substrate and the poly) are negligible and quantum mechanics dominates. As mentioned above, density-gradient theory also has the advantage of having a well-defined connection to the real physics of the problem.

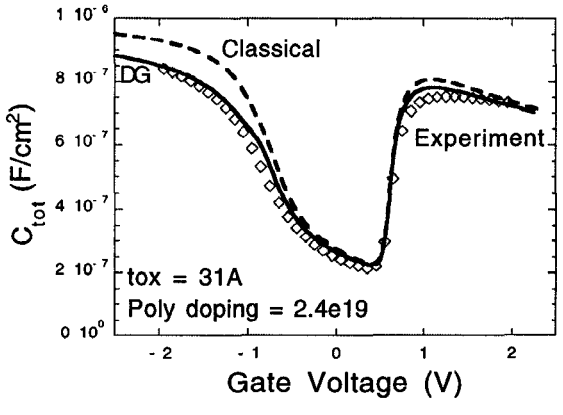


Fig. 4. Comparison of experimental (diamonds) C-V data with theoretical curves with (solid line) and without quantum effects (dashed line). The only fitting parameter in these calculations is the doping level in the poly gate.

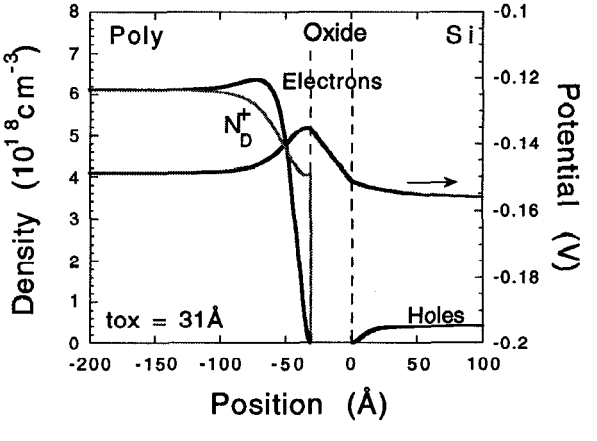


Fig. 5. Density and potential profiles as computed by density-gradient theory for a bias near flatband. Notice the dipole in the poly due to the quantum confinement.

Finally, an interesting phenomenon associated with the quantum exclusion effect may be noted in the carrier profiles near flat-band as plotted in Fig. 5. The quantum exclusion induces a dipole in the near surface region of the poly. The strength of this dipole in our example is given by the height of the potential step in the poly in Fig. 5 (roughly 20mV). This dipole appears to cause a bump in the quantum space-charge capacitance of the gate.

## IV. FINAL REMARKS

In summary, this work demonstrates the utility and power of the density-gradient approach for analyzing equilibrium quantum effects in ultra-thin-oxide MOS structures. This approach not only allows simple yet quantitatively accurate simulation of equilibrium C-V characteristics but, in contrast to the exact alternative [5], can also easily and consistently be extended to multiple dimensions and to non-equilibrium cases including situations with oxide tunneling.

## ACKNOWLEDGMENT

MGA thanks the Office of Naval Research for funding support.

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