On Density-Gradient Modeling of Tunneling through Insulators

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***Abstract*— The density gradient model (DG) is tested for its ability to describe tunneling currents through thin insulating barriers. Simulations of single barriers (MOS diodes, MOSFETs) and double barriers show the limitations of the DG model. As a reference the Schrödinger-Bardeen method is taken. 'Resonant tunneling' in the density gradient model turns out to be an artifact related to large density differences in the semiconductor regions.**

I. Introduction

Quantum effects in modern deep-submicron devices are of growing interest. A prominent unwanted quantum effect in MOSFETs is direct tunneling through the thin gate dielectric, which increases the off-state power consumption. Another important effect is quantum depletion, the carrier density decay towards barriers. In MOSFETs this leads to a shift of the inversion charge maximum away from the oxide interface which in turn causes a shift of the threshold voltage, a lowering of the gate capacitance and an apparent increase of the oxide thickness.

There are several methods that can be combined with conventional drift diffusion simulators to include these effects:

Quantum depletion effects can be accurately modeled by solving the one-dimensional Schrödinger equation along the confinement direction self-consistently coupled with the device equations [1].

Established methods for modeling direct tunneling [2] are the calculation of a transmission coefficient [3] and the use of Bardeen's transfer Hamiltonian [4, 5] with either quasi-classically Wentzel-Kramers-Brillouin (WKB) wave functions or self-consistently obtained numerical solutions of the 1D-Schrödinger equation [1].

An interesting, computational efficient alternative for including quantum effects into conventional device simulators is the density gradient (DG) model. This model introduces a quantum correction term containing higher derivatives of the density or the electrostatic potential into the usual drift diffusion or hydrodynamic device equations [6–9]. The DG model is known to describe quantum depletion effects very well [1]. It also has been applied to one-dimensional insulator tunneling [10] (using two carrier populations according to tunneling direction) and source to drain tunneling in short channel MOSFETs [11].

The aim of this paper is to demonstrate the degree to which the DG transport model is capable of reproducing direct tunneling currents through insulating barriers. As a reference we use simulations solving the one-dimensional Schrödinger equation combined with Bardeen's transfer Hamiltonian method for calculating the tunneling current [1, 4]. All devices studied here are silicon based with single or double SiO_2 barriers.

The DG model and modifications for non-equilibrium are described in section II. Simulations of tunneling characteristics with these models and the reference method are presented in section III. The findings are discussed in section IV.

II. Model

The density gradient (DG) model (or 'quantum drift diffusion', QDD) [1, 7, 9, 12, 13] can be viewed as a modification of the usual drift diffusion (DD) model. A 'quantum potential' Λ is introduced into the classical formulas of the electron density n and the current density $\vec{J}_n$ (we restrict the considerations below to electrons, for holes corresponding expressions exist):

$$n = N_\mathrm{c} \exp\left[\beta\left(E_{\mathrm{F},n} - E_\mathrm{c} - \Lambda\right)\right] \tag{1}$$

$$\begin{aligned}\vec{J}_n &= -\mu\, kT\, \nabla n - \mu\, n\, \nabla(E_\mathrm{c} + \Phi_m + \Lambda) \\ &= -\mu\, n\, \nabla E_{\mathrm{F},n}\ ,\end{aligned} \tag{2}$$

with $\beta = 1/kT$, the electron quasi-Fermi energy $E_{\mathrm{F},n}$, the conduction band edge E_c and a mass driving term $\Phi_m = -kT\log N_\mathrm{c}$ from DOS discontinuities. In the formulation presented here, Λ is the solution of the partial differential equation:

$$\Lambda = -\frac{\gamma\hbar^2}{12\,m}\left[\nabla^2 \log n + \frac{1}{2}\left(\nabla \log n\right)^2\right] \tag{3}$$

$$= -\frac{\gamma\hbar^2\beta}{12\,m}\left[\nabla^2\left(\xi E_{\mathrm{F},n} - \overline{\Phi}\right) + \frac{\beta}{2}\left(\nabla\left(\xi E_{\mathrm{F},n} - \overline{\Phi}\right)\right)^2\right], \tag{4}$$

where $\xi = 1$, γ is a fit factor and $\overline{\Phi} = E_\mathrm{c} + \Phi_m + \Lambda$. Together with Poisson and continuity equation the formulas (1,2,4) form a system that has to be solved self-consistently.

The density gradient model is derived as a moment expansion of the Wigner-Boltzmann [14] or a corresponding quantum Liouville equation [9] and a situation close to thermal equilibrium is assumed. The derivation in [1] calculates an equilibrium solution for the density matrix as a first order perturbation in E_c. Additionally it is assumed that E_c varies only slowly on the scale of the thermal de-Broglie wavelength. The result is a formulation given by (1,2,3) with $\gamma = 1$ where instead of the density n actually the *classical* equilibrium density $n_\mathrm{cl} \propto \exp(-\beta E_c)$ appears in (3). When this is replaced by the *quantum mechanical* density n we obtain (3) with Λ appearing also on the right hand side. This replacement generates a smooth $\overline{\Phi}$ even at band edge jumps $\Delta E_c \gg k_B T$, which violates the assumptions made above, but corresponds to the situation encountered at the Si-SiO$_2$ interface. This step still lacks a satisfactory justification. Nevertheless the DG model is able to describe equilibrium densities in MOS channels very well when compared to a more accurate 1D-Schrödinger solver [1].

'Tunneling' in the DG formulation originates from the reduction of the barrier[1] by the presence of Λ in the current equation (2). The carriers only have to surmount the residual barrier $\overline{\Phi}$. The tunneling current is not separated from the drift-diffusion current and hence is determined by the mobility μ_{ox} in the oxide, which we use as a fitting parameter.

In order to allow for transport modeling a space dependent quasi-Fermi energy is introduced in (4). This expression can be generalized by setting $\xi \neq 1$ [15]. As the derivation of Eq. (3) is valid close to equilibrium only, the proper value for ξ is not known from theory. For tunneling, $E_{\mathrm{F},n}$ varies significantly over the barrier, and the value for ξ matters. Therefore, we examine the cases $\xi_{\text{ox}} = 1$ and $\xi_{\text{ox}} = 0$ in oxide regions. In semiconductor regions, $E_{\mathrm{F},n}$ varies little and we use $\xi = 1$ throughout.

III. Simulations and Results

Single and double barrier devices were studied with the simulation tool DESSIS. The implementation of the density gradient model is described in [15]. As a reference the one-dimensional Schrödinger equation is solved self-consistently coupled to the potential in a region containing the oxide and a part of the substrate next to it. The Bardeen tunneling current is then calculated a posteriori using the resulting numerical wave functions and assuming plane waves in the polysilicon gate [1].

A. N-channel MOSFET

Gate tunneling characteristics (gate current I_{Gate} versus gate voltage V_{GS}) were produced for symmetric n-channel MOSFETs[2] with two oxide thicknesses (Fig. 1). Source, drain and back contact were kept at zero potential.

For $\xi_{\text{ox}} = 1$ and small positive bias ($V_{\text{GS}} \lesssim 0.5$V) one obtains DG curves close to Schrödinger-Bardeen (SB) results by using an oxide mobility $\mu_{\text{ox}} = 0.05$ cm^2/Vs. However, for $V_{\text{GS}} < 0$ there is a strong discrepancy, the most peculiar feature being a current peak very close to 0V and a minimum enclosing a region $-1\text{V} \lesssim V_{\text{GS}} \lesssim 0\text{V}$ where negative differential resistance (NDR) occurs.

Using $\xi_{\text{ox}} = 0$ yields monotonously rising currents, which are, however, too high for positive and too low for negative bias. Hence, fitting μ_{ox} does not improve the situation.

For the 2nm device additional SB simulations have been carried out including a self-consistent current calculation.

[1]The insulator is treated as a semiconductor with a wide bandgap and insulator parameters.

[2]For all simulated devices the term MOS actually implies a highly n-doped (10^{20} cm^{-3}) polysilicon region instead of metal.

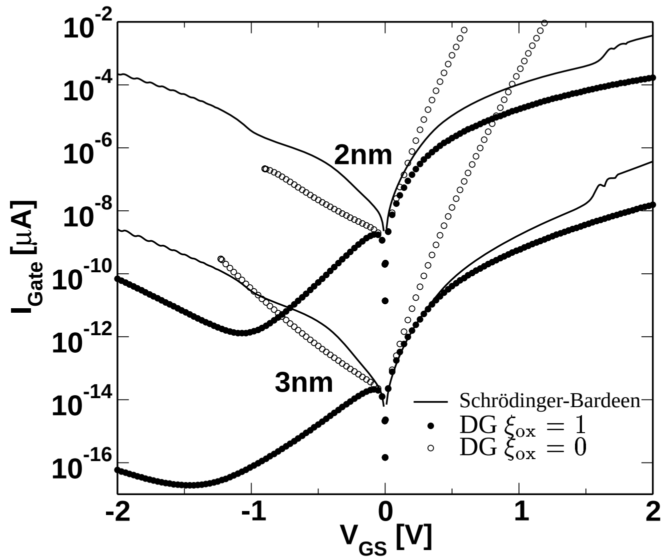

Fig. 1. Gate 'tunneling' currents in n-channel MOSFETs. Density gradient results (symbols) are compared to Schrödinger-Bardeen (lines).

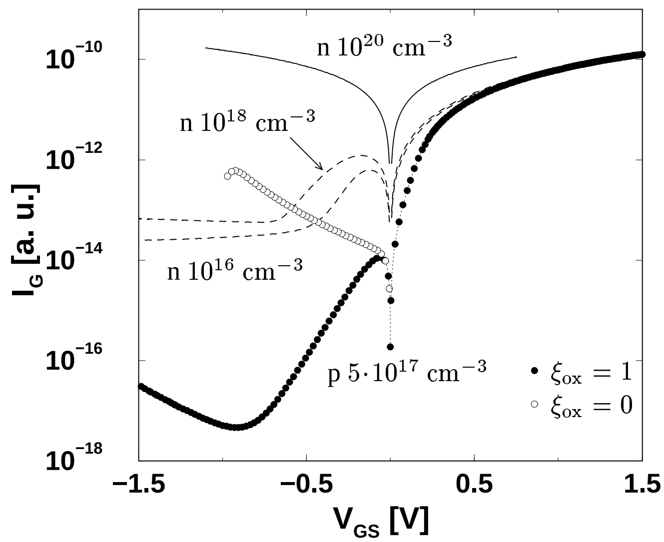

Fig. 2. DG 'tunneling' currents for MOS diodes (structure n$^+$Polysilicon–Oxide–Si) with different Si dopings. All curves are shown for $\xi_{\text{ox}} = 1$ unless indicated otherwise.

Apart from a worse convergence behaviour no difference was found for the current characteristics. The current is too small to add a significant contribution to the substrate space charge.

B. MOS-diode

For a simpler system, a one-dimensional MOS-diode with a 2nm oxide, similar DG current characteristics are obtained as for the MOSFET (symbols in Fig. 2). The name V_{GS} applies now to the voltage at the n$^+$-polysilicon 'gate' contact with respect to the substrate. Here, having no source and drain contact the carrier supply is limited by thermal generation. For a better comparability, the lifetimes of SRH generation/recombination in the substrate were set to extremely small values.

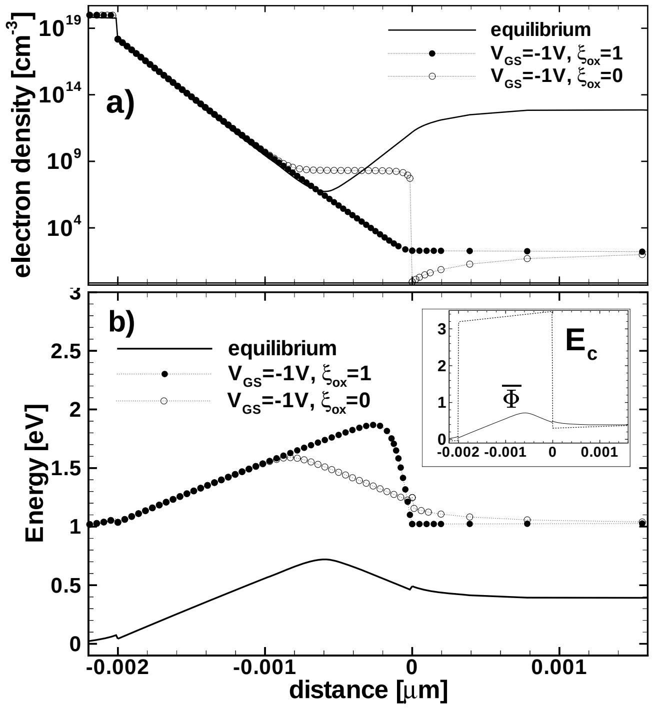

Fig. 3. Electron density n (a) and effective band edge $\overline{\Phi}$ (b) along a MOS diode at different gate voltages for $\xi_{ox} = 1$ (lines) and $\xi_{ox} = 0$ (symbols). The structure (from left to right) is: n^+-Polysilicon—Oxide—Si. The oxide-semiconductor interfaces are located at 0 and -2nm, respectively. The inset in b) shows the equilibrium effective barrier $\overline{\Phi}$ compared to the conduction band edge E_c. The small steps in $\overline{\Phi}$ at the interfaces are due to the DOS discontinuities Φ_m that are not included in this graph.

The electron density n and the residual barrier $\overline{\Phi}$ are shown for $\xi_{ox} = 0$ and $\xi_{ox} = 1$ in Fig. 3a) and b), respectively. The inset in Fig. 3b) compares the conduction band edge E_c with the effective band edge $\overline{\Phi}$ for the case of thermal equilibrium. The barrier is largely reduced. In equilibrium the two cases for ξ_{ox} are equivalent, but with ceasing inversion they exhibit different profiles in the oxide as well as in the substrate region next to it. Most striking is the discontinuity of the density at the oxide-silicon interface for $\xi_{ox} = 0$.

Exploring the case $\xi_{ox} = 1$ for different substrate doping (Fig. 2) we find that the NDR behaviour vanishes for symmetric doping, as expected for a symmetric device structure.

C. *Resonant tunneling diode*

NDR is an effect known to occur in resonant tunneling devices (RTDs). The results with single barrier MOS-structures motivated the investigation of the DG model applied to silicon RTDs with two SiO_2 barriers enclosing a quantum well of varying thickness. The structure is shown in Fig. 4. The well is intrinsic and the outer regions are highly n-doped ($10^{20}\mathrm{cm}^{-3}$). The barriers are 1nm wide. For all following results $\xi_{ox} = 1$ was used.

Current characteristics obtained from DG simulations are shown in Fig. 5 (dashed lines). In addition, a curve for a single oxide barrier between intrinsic and n-doped silicon is included (circles in Fig. 5) which seems to be approached by the double

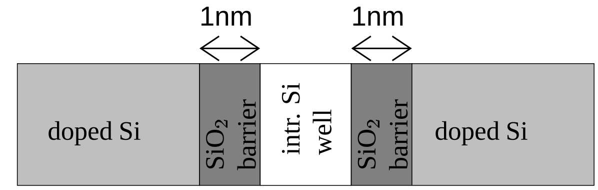

Fig. 4. Structure of a RTD as used in the simulations. The well consists of an intrinsic silicon region sandwiched between two SiO_2 barriers of 1nm width.

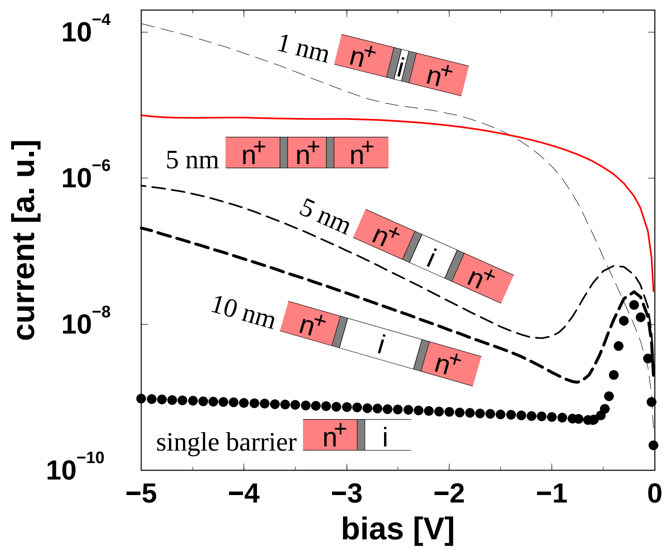

Fig. 5. Currents for RTDs with different well lengths calculated with the DG model ($\xi_{ox} = 1$). The small pictures illustrate the device structure. There are three kinds: The RTDs have an intrinsic well with different lengths (dashed lines, white middle regions). One RTD has a n-doping of $10^{20}\mathrm{cm}^{-3}$ also in the well (solid line, shaded middle region). The third structure is a single barrier MOS-diode with an intrinsic substrate (•).

barrier devices, if the well length is increased. Furthermore, the NDR-like feature vanishes, if the outer regions and also the well are equally n-doped (solid line in Fig. 5).

The existence of the DG current peak and a corresponding NDR is related to the dimension of the intrinsic well region. It is present if the well extends over 5nm or more. For a narrow well, measuring only 1nm, this effect does not appear (thin dashed line in Fig. 5). For this small well length NDR reappears only by switching to p-doping in one of the outer regions, i.e. when the difference in density across the *whole* device is increased, which is shown in Fig. 6 (solid line).

In Fig. 6 characteristics of SB and DG simulations are compared for a RTD having a p-doped and a n^+-doped electrode and an intrinsic well with a length of 1nm. The SB characteristics exhibits two main resonance peaks (symbols in Fig. 6) that are clearly different in number, location and peak value from the single current peak that is obtained for the same device with the DG model (solid line in Fig. 6). Consequently, the DG model can not reproduce the resonance effects of this device.

For the corresponding symmetrically n^+-doped device with an intrinsic well, the peak is absent (dashed line in Fig. 6). As seen before, this is related to the small well dimension. This

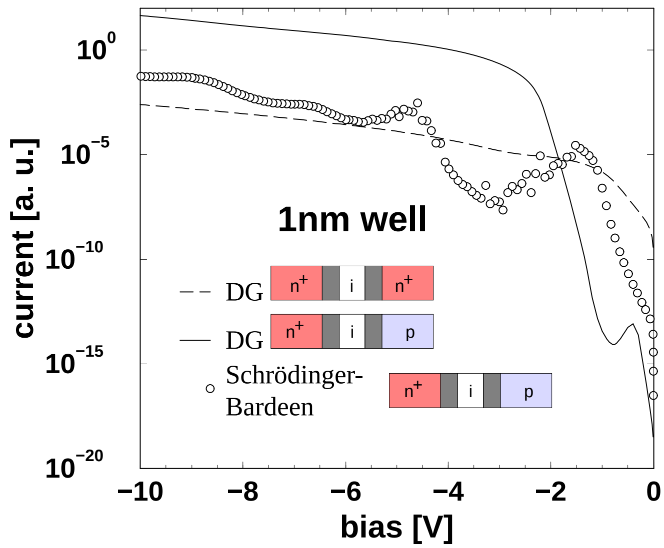

Fig. 6. DG current characteristics for an RTD with asymmetrical (p-i-n^+) doping (solid line) compared to Schrödinger-Bardeen (symbols). A symmetrically doped device (n^+-i-n^+) is also shown (dashed lines). Well and barriers are both 1nm wide.

curve, like for a WKB approximation, shows no resonance but seems to depict an average of the SB characteristics.

IV. Conclusion

The DG model has been used to simulate electron tunneling across oxide barriers in silicon MOSFETs, MOS-diodes and RTDs. The modified model ($\xi_{\mathrm{ox}} = 0$) produces discontinuous carrier densities, if tunneling occurs from high to low density regions. Non-monotonous current-voltage curves are observed for standard ($\xi = 1$) DG simulations of single barrier as well as double barrier structures.

The negative differential resistance vanishes, if both sides of a barrier are symmetrically n-doped or bias conditions are such that high electron densities exist on both sides (inversion). Only in this case a satisfying description similar to the WKB approximation can be obtained. Thus, the presence of NDR-features is related to large density differences across the barrier.

Particularly for RTDs a NDR-like feature in the DG simulation disappears, if all semiconductor regions are equally doped. Furthermore, the resonances of a Schrödinger-Bardeen simulation of a RTD are not related to the DG current peak. Therefore this peak is not related to resonant tunneling. The similarities between single and double barriers also indicate that these features are not caused by quantum interference. They are an artifact of the standard DG model which has to be further examined.

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