Quantum Insights in Gate Oxide Charge-Trapping Dynamics in Nanoscale MOSFETs

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***Abstract*—Charge trapping in the gate oxide of nanoscale MOSFETs featuring an 'atomistic' channel doping profile has been revealed as a key concept to explain the RTN and BTI phenomena strongly affecting contemporary technology transistors performance. By means of a 2D Wigner function approach, in this paper we investigate the trapping of a single electron in the gate oxide of a 25nm transistor including the scattering effects due to discrete dopants in the channel. We demonstrate the ability of our simulation methodology to capture not only the quantum nature but also the transient behavior of charge-trapping and scattering phenomena.**

Keywords—Reliability; Tunneling; Scattering; NBTI; RTN; Wigner Function; charge-trapping; nanoscale MOSFETs

I. INTRODUCTION

Random telegraph noise (RTN) and bias temperature instabilities (BTI) are emerging as major threats to advanced CMOS scaling [1-2]. Recently, experimental and modelling results have helped to identify both RTN and BTI as different manifestations of the same physical phenomenon, namely oxide charge trapping [3-12]. For example, the reliability of SRAM memory cells has been shown to be affected by charge trapping-induced instabilities starting from the 40nm technology node [13]. The importance of these effects increases proportionally to the cell scaling [14-17], advocating for a reliability-aware CMOS design. The latter is virtually unachievable without an accurate understanding of the physics governing the RTN and BTI phenomena, including (i) the effects related to the quantum nature of charge transport and trapping in nanoscale devices [18-19], (ii) the effects of variability induced by the atomistic nature of dopants [20-22], (iii) the transient effects governing the charge transfer of carriers from channel to traps [23]. In this work we present a 2D full-quantum transient simulation study of charge transport in a nanoscale MOSFET including charge trapping/detrapping (t/d) dynamics into the gate oxide and scattering dynamics by discrete dopants in the channel. Phonon scattering is suppressed in the applied Wigner particle model in order to analyse the coherent physics of the trapping/detrapping process. The evolution of an initial electron packet subject to the action of device channel potential and the oxide trap barrier is followed in time. The impact of a single discrete dopant scattering centre on destroying the coherence of the wave

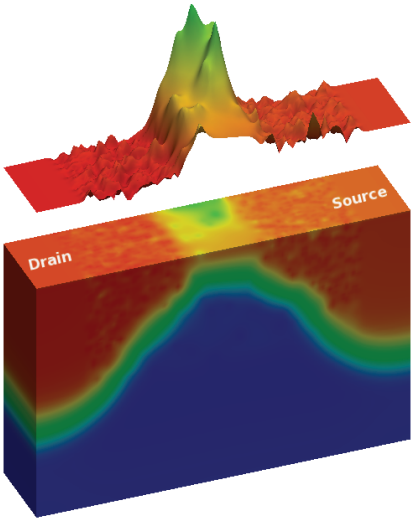

Fig.1 Effective potential for the 25nm 'atomistic' MOSFET investigated in this work (V_G=0.15V,V_D=0.05V).

packet is also separately evaluated. This approach is particularly apt in the statistical limit where the discrete nature of the electron charge does not allow a stationary description: at currents below 10^{-7}A single electrons are injected at time intervals larger than one picosecond. Alternatively the electron may be considered as just released from another trap in the channel. However general injecting boundary conditions for channel electrons can be accounted by our model. Our study demonstrates the feasibility of a 2D Wigner particle simulation methodology in capturing not only the quantum nature but also the transient behavior of charge-trapping and scattering phenomena. This approach can be used to evaluate the dependence of the charge capture time – e.g. defined as in [24] – on the trap shape, surrounding channel potential profile and electron packet parameters. Furthermore statistical fluctuations in the gate potential can also be investigated as they influence the capture time due to the exponential dependence of the tunnelling probability on the trap barrier height. We also show that, due to the non-locality of the quantum potential, the effect of a discrete dopant exceeds the classically expected behavior, and in particular can block the closest to the interface part of the channel for transport of electrons.

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II. Simulation Methodology

In order to obtain a realistic potential profile of a nanoscale device, we have performed 3D simulations of a well-scaled 25nm MOSFET device using the GSS 'atomistic' simulator GARAND [25]. Fig.1 shows the effective potential in the presence of a discrete trap and discrete random dopants. A vertical slice of the 3D device is then extracted and used to perform a 2D Wigner simulation of the charge transport in presence of discrete traps and discrete dopants. The trap is introduced by means of an approximated 2D squared quantum well at the channel/oxide interface. The quantum transport is obtained by using a modified version of Archimedes (nano-archimedes), which implements the Wigner Monte Carlo method [26]. The Wigner Monte Carlo method is a time-dependent full quantum transport model which naturally includes both open and closed boundary conditions along with general initial conditions. In contrast to classical particles driven by the first derivative of the electric potential, quantum particles feel all other derivatives, as can be shown by the Taylor expansion of the Wigner potential [27]. This is a manifestation of the non-locality of the quantum electron-potential interaction. Instead of a classical acceleration over Newton's trajectories by the local field inherent for the classical Monte Carlo approach, the action of the Wigner potential on the quantum particles representing a single electron is by generation of particles with opposite sign, locally in the position and following certain rules in the momentum component of the phase space. Thus signed particles evolve over field-less Newton's trajectories and contribute to the values of the physical averages by their sign. Thus two particles with the same phase-space coordinates but opposite signs compensate each other, or annihilate. The quantum transport picture comprises generation and annihilation at consecutive time steps of signed particles [28]. The process of annihilation reduces the particle number and actually makes it possible to extend quantum particle approaches beyond one-dimensional applications.

III. Results and Discussion

A. Charge trapping in gate oxide

The simulation consists of an initial 2D Gaussian wave packet with initial energy equal to ~0.15eV and an initial velocity oblique to the direction of the silicon oxide. The trap inside the oxide is of rectangular shape with zero bottom energy. A high barrier is placed at the interface between the channel and the oxide with energy equal to 1.5eV. Thus, a packet can enter the trap zone only by quantum tunnelling process. Fig.2 (a-e) shows the dynamics of the wave packet. At 1fs (b) the degradation of the wave packet due to the channel potential is already visible, at 2fs (c) the trap starts to be charged, and at 3fs (d) the trap is occupied as above 1% of the initial density is already inside it. Finally, at 4fs (e) the wave packet is already bouncing back.

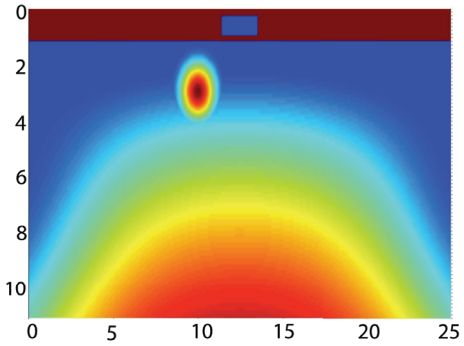

Fig.2.a initial Gaussian wave packet. The oxide thickness is 1.2nm, the trap area is 2x0.6 nm^2. The tunnelling barrier thickness is 0.2nm, the rest of the interface is treated classically.

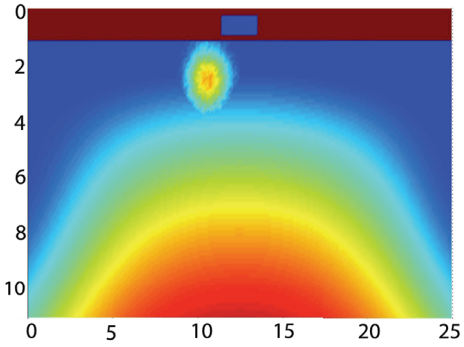

Fig.2.b The channel potential is starting to destroy the smoothness of the packet and at around 2fs the charging of the trap begins (compare with Fig.3).

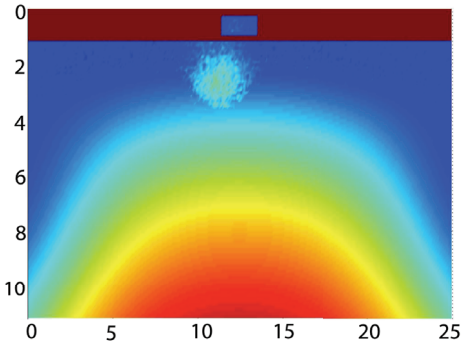

Fig.2.c At 4fs the wave packet already bounces back and decoherence starts to appear. Nevertheless the appearance of trapped components of the packet presented by the green dots well visible in the trap region, compare with Fig.2.b.

In Fig.3 we show the accumulation of the normalized trapped charge, with respect to the total charge, as a function of time.

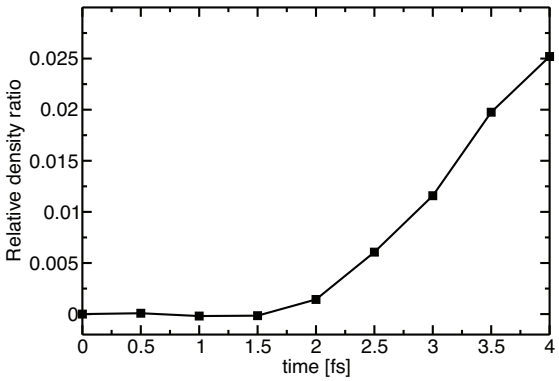

Fig.3 The time-dependent relative ratio between the trapped and travelling densities shows insight about the charging time.

B. Scattering by single dopants

In the previous section we have considered the wave packet evolving in an idealistic smooth potential provided by 3D TCAD simulations featuring a continuous doping profile. However, only a handful of dopant atoms lays inside the active region of a nanoscale transistor determining a potential far from uniform [29-30]. Each of these dopants acts as a scattering centre breaking the phase coherence of the wave packet. Therefore, in this section we evaluate the impact of a single 2D δ-like barrier with energy 0.5 eV and width 0.3 nm and distant 0.4 nm from the oxide interface. The 2D Gaussian wave packet initial conditions for the experiment shown in Fig.4 are the same as in Section III.A. Two main phenomena are emerging: (i) the spread of the packet behaves differently, the evolution is retarded, compare Fig.2.b with Fig.4.b, the effect is more pronounced between Fig. 2c and Fig. 4c; (ii) the scattering is felt across the channel well around the center position. Indeed the Boltzmann evolution can be easily anticipated and used as a reference. |The whole palette of package colors will surround the centre. Only particles in the proximity will be affected, namely only those hitting the surface will be scattered back. In contrast the vicinity of the centre remains rarely populated even after 8fs, Fig.4.d and especially the region between the centre and the interface with the oxide. This part of the channel remains blocked due to non-local quantum effects except for very low densities: we note that the interface is treated classically, which in particular avoids interference effects with the scattering centre potential. Moreover the quantum interaction effectively destroys the far end of the packet, showing that actually it affects the transport in the whole cross section of the channel. In other words, the quantum non-locality makes the interaction with the scattering center a prominent effect which eventually reduces the current in the device (as it is experimentally observed – degradation of the device performance).

IV. Conclusions

We have studied the evolution of a wave packet in a nanoscale MOSFET featuring discrete oxide traps and discrete channel dopants. Our 2D Monte Carlo Wigner simulation approach is able to capture both the quantum and the transient nature of

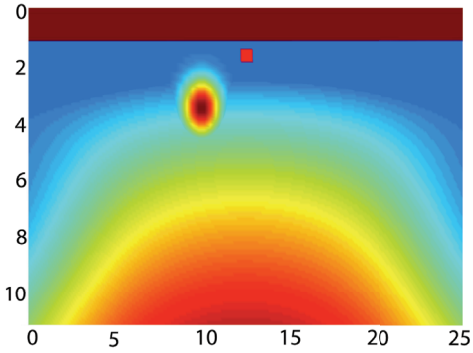

Fig.4.a Evolution of a Gaussian wave packet in proximity of a scattering center at 1fs. The packet is already starting to spread.

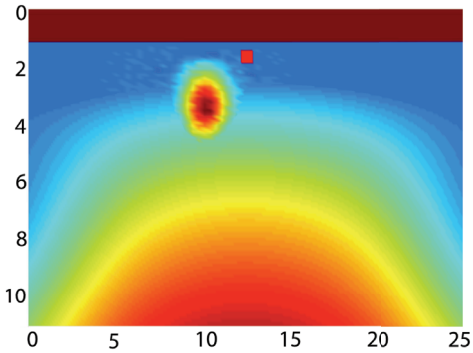

Fig.4.b At 2fs the evolution is retarded as compared to Fig.2.b. Forth and back scattered components begin to form.

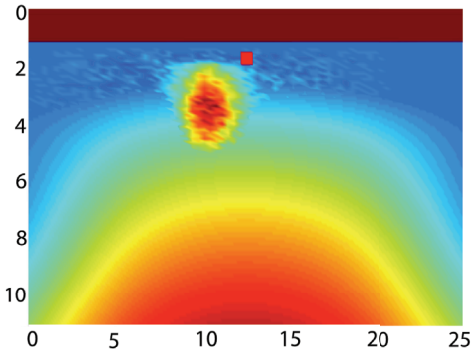

Fig.4.c At 4fs the packet destruction is in progress.

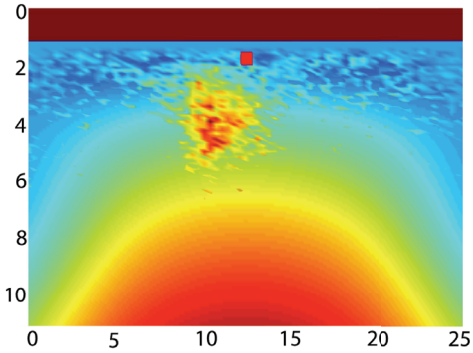

Fig.4.d The centre is felt by the far end of the packet.

charge-trapping and scattering phenomena. Based on this technique, we suggest the charging time can be obtained by averaging different packets having parameters, such as initial position, velocity and shape, taken from boundary conditions pre-calculated by semi-classical methods. The quantum effects due to the presence of a scattering centre are manifestly nonlocal: the electrons are affected outside the geometric limit of the centre, in particular the part of the channel between the centre and the interface remains blocked for transport, which is in a deep contrast to the envisaged behaviour of classical Boltzmann electrons.

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