Coupled Monte Carlo Simulation of Si and SiO_2 Transport in MOS Capacitors

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Abstract— **We present a Monte Carlo (MC) model comprising SiO_2 and Si transport, suitable to simulate carrier multiplication in MOS structures. The code extends full-band density of states (DoS) and scattering rate calculations in silicon up to high energy. Simulations of 5-15 nm oxides for Non Volatile Memory applications demonstrate the role of oxide transport on the distribution of the holes generated by impact ionization, which are often regarded as the origin of oxide degradation, SILC and breakdown.**

I. Introduction

Carriers emerging from oxide to silicon during tunnel experiments in MOS capacitors feature very high energy and give rise to a number of relevant hot carrier effects, e.g. impact ionization (II), quantum yield (QY) [1], and photon emission [2]. Modeling these phenomena is becoming an important ingredient of CMOS and Non Volatile Memory (NVM) reliability studies [3]. Significant efforts were recently devoted to couple impact ionization models and quantum yield analysis to percolation models, and to predict ultra thin oxide reliability [3], [4]. Most of these studies, however, focused on the low quantum yield, low energy, direct or possibly trap assisted tunneling injection regime [5]. Consequently, injected electrons were modeled as a mono-energetic (δ-like) distribution. With the exception of [6], very limited effort has been devoted so far to analyze the high quantum yield measured on relatively thick oxides (5-15 nm), such as those of interest for non-volatile memory applications. In this context, we present an extended Monte Carlo transport model suitable to handle Si-SiO_2-Si gate stacks and demonstrate the impact of oxide transport on the energy distribution of impact ionization generated holes.

II. Silicon transport model extension

Full-band calculations based on non-local pseudopotential theory were extended up to 12 eV by using eight conduction bands instead of the usual four. Electron and hole II scattering rates (S_{II}) and secondary carrier distributions were also extended following the approach of [7] and employing a $\vec{k}$ independent matrix element which yields the same electron and hole scattering rates of [8] at low energy.

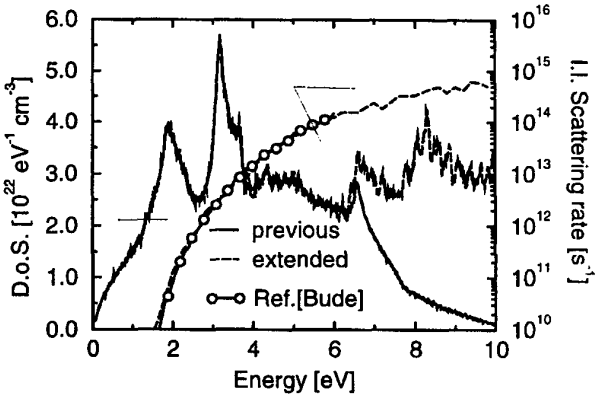

Fig. 1. Electron D.o.S. and impact ionization scattering rate computed up to high energy from non-local pseudopotential theory using 4 (previous) and 8 (extended) conduction bands.

Fig. 1 shows the extended electron density of states (DoS) and the corresponding impact ionization scattering rate (S_{II}) and demonstrates the role of the highest conduction bands for $E > 6$ eV. Fig. 2, instead, reports the calculated secondary carrier distributions for a few energies of the impact ionizing electron. This extension is an important step to properly simulate very high energy carriers such as those emerging at the anode during tunnel experiments and responsible for quantum yields above one.

III. Silicon dioxide transport model

Oxide transport is modeled as in crystalline α-quartz (i.e. neglecting long range disorder) by means of a spherical, non-parabolic band ($m^*_{ox} = 0.5m_0$, $\alpha = 0.2$ eV^{-1}) fitted to the full band structure calculations of [9], [10]. Scattering mechanisms include polar-LO phonons ($\hbar\omega =$ 63 and 153 meV), non-polar acoustic phonons and impact ionization (II). The non-polar acoustic phonon rate and the impact ionization model are the same as in [11].

Fig. 3 demonstrates that average energy versus oxide field (F_{OX}) curves in homogeneous silicon dioxide slabs agree well with [11] and with the experiments of [12].

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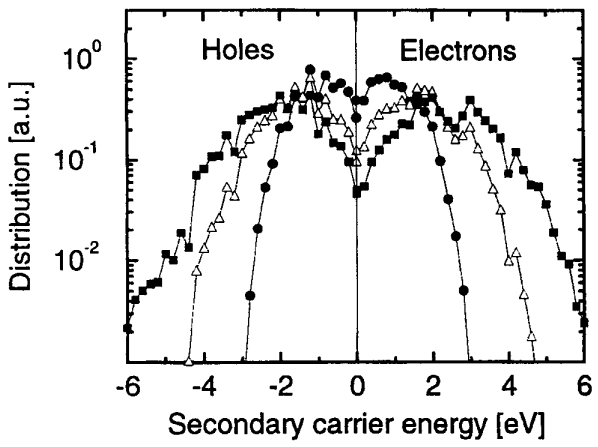

Fig. 2. Normalized energy distribution of secondary electrons and holes generated by electrons at 4 eV (circles), 6 eV (triangles) and 8 eV (squares) in silicon.

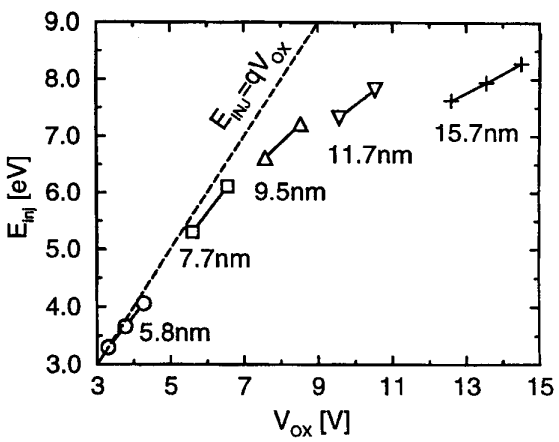

Fig. 4. Average energy of electrons injected from the oxide into the silicon as a function of the voltage drop experienced while traveling in the oxide.

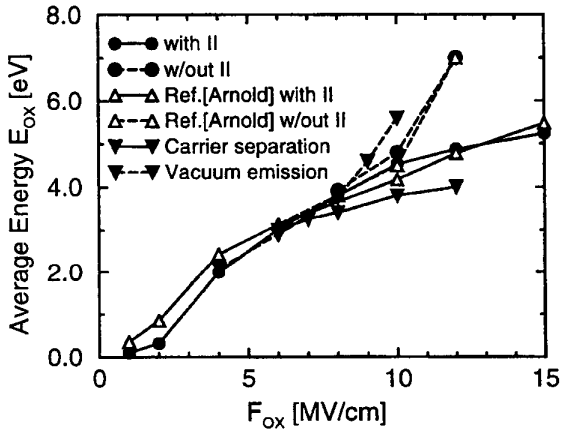

Fig. 3. Average electron energy in the oxide as a function of oxide field with and without impact ionization from simulations of uniform samples according to the model of this work (filled circles), that of [11] (open triangles) and measurements.

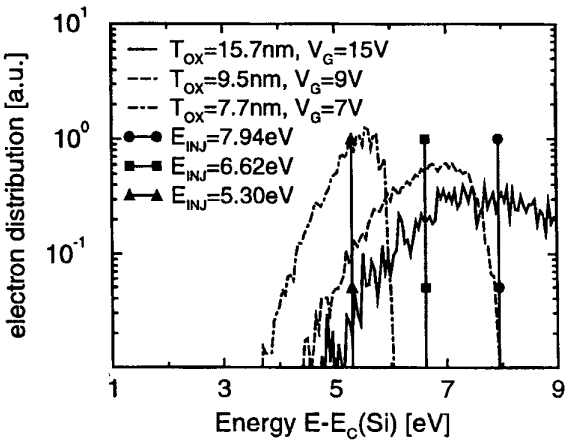

Fig. 5. Electron distributions at the oxide-silicon interface for $T_{OX} = 15.7$ nm, $V_G = 15$ V (solid), $T_{OX} = 9.5$ nm, $V_G = 9$ V (dashed), $T_{OX} = 7.7$ nm, $V_G = 7$ V (dot-dashed). The corresponding average energies E_{inj} are marked by vertical lines.

IV. Simulation Procedure

A fixed electron current (J_G) is generated at the tunneling exit point in the oxide with zero perpendicular energy. The starting electron energy is computed accounting for carrier quantization at the cathode. Parallel momentum conservation of electrons entering silicon is neglected because of the large number of final states available at high energy. Impact ionization generated holes are also simulated, and injected back into the oxide if they hit the interface. The hole tunneling probability (T_h) is computed with the transfer matrix method. A short simulation time step ($\Delta t \approx 0.1$ fs) is needed for an accurate treatment of transport and scattering in the high oxide field.

V. Calibration

Model calibration follows an approach complementary to that of [13]. Namely, electron and hole II scattering rates in silicon are kept the same as in previous works and simply extended to higher energy as described in section II. These rates agree with previous reports [8], [14], and with a large set of experiments on MOSFET substrate current [15] and BJT multiplication coefficient [16]. Therefore,

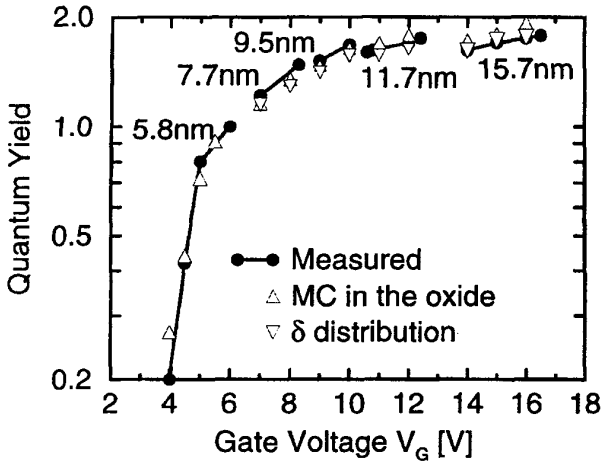

Fig. 6. Comparison between measured Quantum Yield (solid line [5], [1], [13]), MC simulations including oxide transport (triangles up) and simulations injecting electrons according to a δ distribution featuring the same average energy of the MC (triangles down).

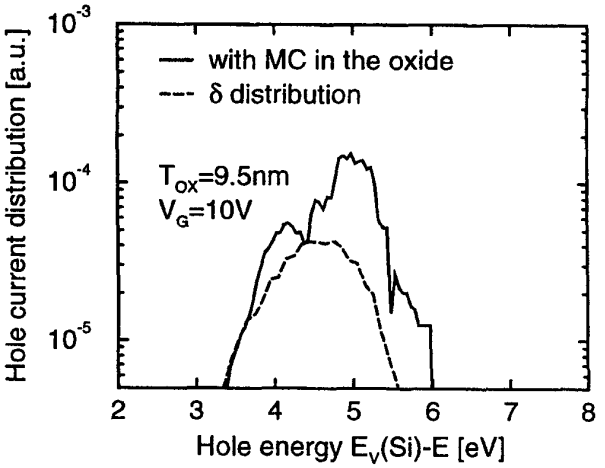

Fig. 7. Energy distribution of holes injected in the oxide (i.e. product of the hole tunneling probability times the hole distribution at the interface) with (solid) and without (dashed) inclusion of oxide transport in the model.

we adjust only the non-polar acoustic phonon coupling contants to improve agreement with the SiO_2 average energy data in Fig. 3.

VI. Results

Fig. 4 reports the average energy of electrons injected from SiO_2 into Si (E_{inj}) as a function of the voltage drop they experienced while traveling in the oxide (V_{OX}). Due to the large oxide phonon's energy and scattering rate, E_{inj} is $\approx$ 200 meV lower than qV_{OX} even in a relatively thin (5.8 nm) oxide. The discrepancy becomes much larger (up to a factor of 2) in 8-15 nm oxides.

Furthermore, oxide scattering broadens the distribution of electrons entering the silicon so that a large number of electrons is injected with energy higher than the average energy E_{inj} even in relatively thin oxides. This effect is displayed in Fig. 5 that compares the actual distribution of injected electrons in a few oxides with the corresponding average energy.

Fig. 6 demonstrates that the model agrees well with quantum yield experiments of thin and thick oxides. For the sake of comparison, simulations were also run injecting electrons directly into the silicon with a δ-like distribution at E_{inj}. We see that quantum yield data is always insensitive to this model simplification, in agreement with findings of [5] limited to low E_{inj}. However, the high energy tail of the hole distribution is significantly affected by the broad range of injection energies generated by oxide scattering. As a result, (see Fig. 7) the distribution of holes

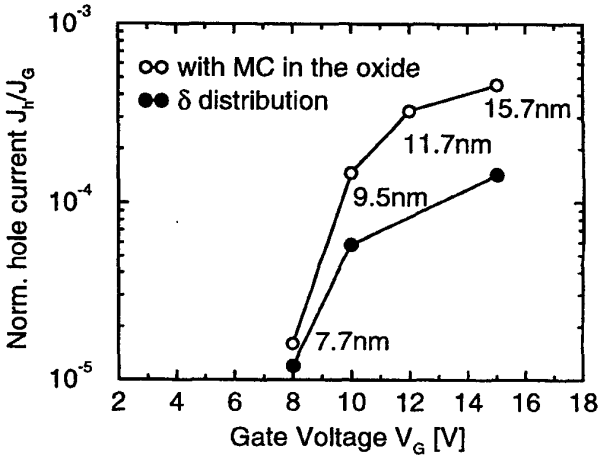

Fig. 8. Ratio between the hole current injected back in the oxide (J_h) and the corresponding electron current J_G in MOS capacitors featuring T_{ox} = 7.7, 9.5, 11.7 and 15.7 nm.

injected back in the oxide (i.e., the product of the hole distribution at the interface by the hole tunneling probability) is strongly enhanced by oxide transport with respect to the case of δ-like injection. This result is confirmed by data in Fig. 8, demonstrating that the ratio between the hole current injected back in the oxide (J_h) and the originating tunneling electron current (J_G) can be reduced by up to a factor of four if oxide transport is neglected.

VII. Conclusions

In summary, a new fully bipolar Monte Carlo code has been developed to simulate hot carriers in MOS capacitors biased in the tunneling regime. The silicon transport model has been extended to high energy and coupled to oxide transport. The model reproduces QY data of thin as well as thick oxides. Simulations demonstrate a significant broadening of the distribution of electrons injected into the silicon, also in relatively thin oxides. This broadening affects the high energy tail of the distribution of anode-generated holes impinging upon the Si-SiO_2 interface, which are often considered responsible of oxide damage in modern CMOS and non volatile memory technologies [3], [4].

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