Electron Transport in Semiconductor-Insulator Structures Using the Full-Band Dispersion Relation of Si and SiO$_2$

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Abstract

Aim of this work is to present a novel simulation tool based on the deterministic solution of the Boltzmann transport equation for electrons in the whole semiconductor-insulator structure. Full-band density of states and group velocity for SiO$_2$ have been incorporated, allowing for an accurate description of the distribution function on an extended range of energies.

1. Introduction

It has been demonstrated that the analysis of high-energy electron transport in Si-SiO$_2$ structures is important for the understanding of the generation of high-energy holes in Si, which are in turn responsible for oxide charge-trapping, degradation and SILC mechanisms [1]. For the electron injection in SiO$_2$, an accurate description of transport both in Si and SiO$_2$ is also important to predict the effect of back-scattered electrons at the interface [2]. To accurately describe the microscopic mechanisms involved in carrier transport, two different approaches may be followed, namely, the Monte Carlo analysis or the deterministic solution of the Boltzmann Transport Equation (BTE) based on the spherical-harmonics expansion (SHE). In this work, the latter is adopted to solve the transport problem in the whole semiconductor-insulator structure. To this purpose, a numerical full-band model for SiO$_2$ has also been developed.

2. The transport model in silicon

The SHE solver incorporates the silicon density of states and group velocity calculated from a full-band structure based on the pseudopotential theory, up to 5 eV. The scattering mechanisms considered are acoustical- and optical-phonons, ionized-impurities, and impact ionization. This physical model allows one to reproduce the bulk carrier transport properties as a function of the electric field, doping concentration, and temperature [4]. The model also accounts for the two-dimensional surface-scattering mechanisms, that in MOS devices are fundamental for the description of mobility degradation at the Si-SiO$_2$ interface. More specifically, the surface-roughness effects have been modelled, as well as the surface-face phonons and Coulomb interaction at the interface [5]. The calibration of the surface effects has been carried out basing upon the universal curves of the effective mobility as a function of the effective transversal electric field $E_{\text{eff}}$.

3. The transport model in silicon dioxide

The analysis of carrier transport in SiO$_2$ is based on the assumption that the amorphous phase exhibits a number of electronic properties similar to those of the crystalline forms of the material. Thus, the numerical full-band structure of $\beta$-cristobalite has been adopted neglecting the long-range disorder of the amorphous phase. The band structure has been calculated by means of the density-functional theory (DFT). The crystal orbital functions have been optimized and eight conduction bands have been used, so that the band structure is accurately described up to 10 eV [6]. The corresponding density of states and group velocity for the conduction band are shown in Fig. 1. The usefulness of a precise description of the band structure at high energies is apparent from the comparison with the analytical-band case.

The scattering models include the polar longitudinal-
optical phonons ($\hbar\omega = 62$ and $155$ meV), the non-polar acoustic phonons, and the transversal-optical phonons ($\hbar\omega = 124$ meV). Coulomb scattering and impact ionization have not been included, as the former has been found negligible in SiO$_2$ [7], and the latter has no influence on the transport in SiO$_2$ up to about 9 eV [1]. The physical parameters in the scattering models have been determined by comparison with Monte Carlo results and with a number of experiments on the carrier average energy, drift velocity and low-field mobility in SiO$_2$ [8]. In Fig. 2, the electron-density distribution in energy of a homogeneous bulk SiO$_2$ structure at different electric fields is compared with that obtained from the spherical-band model of [9]. It is seen that the curves agree only up to 2 eV, whereas they significantly deviate at higher energies.

4. The Si-SiO$_2$ interface

The SHE equations are solved in both the semiconductor and insulator regions. At the interface, two problems have been faced: first, the discontinuity of the potential energy due to the barrier between the two materials; second, the difference in the band structure and scattering mechanisms. Due to the energy barrier, the equations used in a bulk material are not acceptable at the interface because they are based on the first-order truncation of the spherical-harmonics expansion. For this reason, the microscopic fluxes at the interface are calculated basing on the thermionic-emission theory [9]. Due to conservation of energy and parallel momentum, the injection of electrons into the gate oxide is limited within an angular range of the momentum vector. As the models for tunneling and image-force are not included yet, the amount of carrier injection is expected to underestimate the experiments. Nevertheless, the availability of the distribution function on both sides of the interface provides a sound basis for further improvements as those mentioned above.

5. Results and conclusions

To test the physical model at the interface and inside the insulator region, the experiment performed by Ning [10] has been simulated. A MOS transistor was used for the experimental measurement of the gate current. The cross-section of the device is reported in Fig. 3. A suitable electron concentration has been imposed at the substrate contact to simulate the optically-generated electrons of the experiment ($n < 10^{10}$ cm$^{-3}$). The emission probability is calculated as the ratio between the gate current and the sum of source and drain currents. The emission probability calculated by the SHE model as a function of $V_{SB} = -V_B$ for a wide range of gate biases is shown in Fig. 4. The simulated characteristics show a strong dependence on $V_{SB}$. An increase in the latter, in fact, enhances the electric field experienced by the electrons in the bulk. Moreover, the injection of highly-energetic electrons from bulk to gate correctly shows a saturating dependence on the applied gate voltage when the device reaches the complete inversion regime, as no dependence on the shape of the barrier is present there. Since tunneling is not been taken into account, the emission probability is strongly underestimated with respect to the experiments. Figs. 5 and 6 report the distribution function along the cross-section at the middle of the channel obtained at two different electric fields $E_{ox}$ within the oxide and different injection regimes. Fig. 5 refers to the case $E_{ox} = 5.7 \times 10^5$
Figure 4. Emission probability as a function of the bulk voltage at different gate biases. Experiments are by Ning [10].

V/cm ($V_G = 1$ V) and $V_{SB} = 19$ V. Since the device is biased in the subthreshold regime, the distribution function within the silicon region is made only of high-energy electrons coming from the bulk, and shows that their concentration at the interface is small ($5.5 \times 10^{11}$ cm$^{-3}$). The oxide concentration at the interface is 1.1 cm$^{-3}$ as opposed to the equilibrium value $1 \times 10^{-30}$ cm$^{-3}$, suggesting a large electron injection: the corresponding emission probability is $4.5 \times 10^{-9}$. Inside the oxide, the distribution function heats up significantly due to the high electric field. The drop at the gate contact is due to the equilibrium boundary condition, and does not alter appreciably the solution inside the insulator.

In Fig. 6 a different regime is considered: a higher gate bias is applied ($V_G = 6$ V) showing a higher surface concentration (the distribution function at the interface is dominated by equilibrium carriers up to about 1 eV), whereas the electric field in the bulk is lower ($V_{SB} = 6$ V). Thus, the electrons from the bulk reach the surface with a lower energy and the carriers injected into the gate oxide are fewer: the concentration difference across the interface is larger than in the previous figure. The dependence on $V_{SB}$ of the mean energy and carrier concentration inside the insulator can be analysed by fixing the gate bias and changing the $V_{SB}$ (Figs. 7 and 8). The electron temperature normalized to 300 K inside the SiO$_2$ is strongly dependent on $V_{SB}$, due to the heating experienced in the bulk region. In the channel, the normalized temperature is almost equal to 1 because of the large number of equilibrium electrons. Also the electron concentration depends strongly on the bulk bias (Fig. 8): the variation is about five orders of magnitude. Finally, the electron drift velocity at the interface is shown in Fig. 9: as a high electric field is applied to the gate oxide, the drift velocity is saturated in the oxide and is independent of $V_{SB}$.

Figure 5. Energy-distribution function in the middle of the channel as a function of position from gate to bulk. Position 0 corresponds to the gate contact, the Si-SiO$_2$ interface is at 0.0428 µm. Bias conditions: $V_G = 1$ V, $V_{SB} = 19$ V.

Figure 6. Energy-distribution function in the middle of the channel as a function of position from gate to bulk. Position 0 corresponds to the gate contact, the Si-SiO$_2$ interface is at 0.0428 µm. Bias conditions: $V_G = 6$ V, $V_{SB} = 6$ V.
Figure 7. Electron normalized temperature in the middle of the channel as a function of position from gate to bulk. Negative position coordinates correspond to SiO$_2$, positive coordinates to Si. $V_G = 6V$.


Figure 8. Electron concentration in the middle of the channel as a function of position from gate to bulk. Negative position coordinates correspond to SiO$_2$, positive coordinates to Si. $V_G = 6V$.

Figure 9. Electron drift velocity in the middle of the channel as a function of position from gate to bulk. Negative position coordinates correspond to SiO$_2$, positive coordinates to Si. $V_G = 6V$. The spike next to the gate contact is due to the equilibrium boundary condition at the gate.