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Models for the use of commercial TCAD in the analysis of silicon-based integrated biosensors

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ABSTRACT

We present a simple approach to describe electrolytes in TCAD simulators for the modeling of nano-biosensors. The method exploits the similarity between the transport equations for electrons and holes in semiconductors and the ones for charged ions in a solution. We describe a few workarounds to improve the model accuracy in spite of the limitations of commercial TCAD. Applications to the simulations of silicon nanowire and nano-electrode biosensors are reported as relevant examples.

1. Introduction

The development of nanoscale semiconductor devices as sensing elements for the detection of biological species represents a promising and exciting field of application for CMOS technology in the More-than-Moore domain. Biosensors for liquid environments often consist of a conventional MOSFET, where the gate is replaced by an electrolyte forming the so-called *fluid-gate* [1]. The target molecules diffuse in the electrolyte toward the gate dielectric, where they bind with the receptors, thus perturbing the charge density on the gate and modifying the threshold voltage and the conductance of the device.

The sensitivity of such a biosensor is strongly degraded by dielectric screening, i.e. the ions in the electrolyte arrange themselves to screen the charge of the target molecules [2]. Unfortunately, for most analytes employed in real experiments, the ion concentration in the electrolyte cannot be reduced below a minimum level without affecting the properties of the target molecules and impeding their binding to the receptors.

Models for the electrolyte in the continuum are typically based on the solution of the Poisson–Boltzmann (PB) equation by means of ad-hoc simulation codes that are applicable to a restricted set of simple template structures [3–6]. However, to be useful for the design and optimization of integrated electronic biosensors, numerical models should incorporate a general description of the semiconductor device and, at least, a first order description of the biomolecules and their environment. Available commercial TCAD is not equipped to model electrolytes or buffer solutions. On the other hand, TCAD offers detailed and accurate models for the semiconductors and the capability to handle complex and arbitrary device geometries.

In order to expand the applicability of TCAD to biosensors, this work describes a simple technique to include an "electrolyte material" region into the commercial TCAD simulator SDevice [7]; this approach trades a simplified description of the electrolyte for the possibility to exploit the above mentioned pros of the TCAD[1] without embarking in the costly development of ad-hoc codes.

The paper proceeds as follows: Section 2 presents the simulation approach, which is then applied to nanowire biosensors in Section 3. The limit of the PB equation and the importance of steric effects are analyzed in Section 4 with reference to nano-electrodes based biosensors. Section 5 is devoted to the analysis of the choice of permittivity of the compact layer, while Section 6 addresses the approximations inherent to the TCAD in modeling complex multi-ion electrolytes. Conclusions are reported in Section 7.

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[1] Some of the results in this manuscript have been already reported in Palestri et al., Proc. ULIS 2013. In the present manuscript we extend the analysis by adding results for a 3D nanowire and by analyzing in more detail the influence of steric and interface effects.

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2. Model description

We exploit the similarity between the equations describing positive and negative ions in the electrolyte and those for holes and electrons in a semiconductor. In this respect, a 1:1 electrolyte can be described in SDevice as a semiconductor (that we call "electrolyte material") with zero gap, a constant permittivity[2] and an effective densities of states in conduction and valence band:

$$N_C = N_V = N_A c_0 \times 10^{-3} \tag{1}$$

where N_A is Avogadro's number and c_0 the ion molar concentration (M = mol/l) in the bulk of the solution, defined as a region where we have the same concentration of positive and negative ions, hence overall charge neutrality.

The electron and hole mobility in this "electrolyte material" is adjusted to the corresponding values of the ions [8]. Care should be paid to disable the default temperature dependence of the model parameters and to avoid the build-up of unphysical offsets in N_C, N_V, E_G and mobility whenever the temperature is different from the model reference value.

The proposed approach allows us to easily exploit all the features of the TCAD, such as: calibrated mobility models for silicon, multiple type of analysis and the handling of arbitrary geometries in 2D and in 3D. Clearly, there are limitations as well. First of all, only a single 1:1 ionic solution can be included, whereas electrolytes with many types of ions and diversified valence are used in experiments; this point will be discussed later in Section 5. In addition, only idealized interfaces without steric effects [9] and without surface reactions [10] can be treated. The control on the numerical error is also quite limited with respect to ad-hoc codes developed for the modeling of electrolyte screening, such as for instance [3].

An approach similar to the one proposed here has been recently, but independently, reported in [11]. In the present paper we go well beyond the model in [11] by proposing strategies to account for steric effects, solutions with multi-ions and polarizability effects of the water at the interfaces.

3. Application example: sensing biomolecules with nanowires and nanoribbons

As an example, we consider a biosensor inspired by the nanoribbons presented in [12]. In virtue of the large width we consider a 2D simulation domain. We assume full coverage of the gate oxide by the target molecules and by the receptors; these are modeled as a 5 nm thick dielectric layer with a volume charge density corresponding to 10^{12}–10^{13} cm^{-2} charges per unit area, that is, approximately 10 unit charges per molecule and 10^{11}–10^{12} molecules per cm^2, consistently with the estimates for molecules such as avidin and streptavidin bound to biotin reported in [13]. The dielectric constant in the layer is known to be much smaller than that of the electrolyte and is tentatively set to $2\varepsilon_0$.

The simulated structure is sketched in Fig. 1 and is a p-type gated resistor (as in [12]).

Fig. 2 reports the relative change of conductance induced by a density of elementary charges σ (number of electrons per unit area[3]) with respect to the case where the dielectric layer is not charged. In other words, we are implicitly assuming that the receptors are initially not charged and that the arrival of the target molecules changes the charge in the 5 nm layer of Fig. 1. We see that the sensitivity of the sensor changes with the bias and it is larger for close-to-zero or, even better, for slightly positive back-gate bias. In fact, since the device is essentially a gated p-resistor, it becomes more sensitive to charge variations when the channel is depleted of holes. For low σ values, the sensor sensitivity characteristic is symmetric for positive or negative σ. At large σ values, the sensor gets more sensitive to positive charges since they further deplete the channel.

Fig. 3 reports the device sensitivity for different doping levels in the channel; as expected, with low doping the conductance becomes more sensitive, since the charge of the target molecules efficiently depletes (or accumulates, depending on the charge sign) the hole-rich channel. Fig. 4 shows that the sensitivity can be enhanced by using thin channels.

The results in Figs. 3 and 4 can be explained considering that the perturbation induced by the charged molecules on the hole concentration in the silicon ribbon exponentially decays in space with a characteristic length given by the Debye length:

$$\lambda_D = \sqrt{\frac{\varepsilon_{Si}\varepsilon_0 k_B T}{q^2 p}} \tag{2}$$

where p is the hole concentration in the wire, implicitly assumed to be uniform. λ_D is close to 12 nm for $p = 10^{17}$ cm^{-3}. The sensitivity is larger when λ_D is in the order of T_{CH}, because the ribbon tends to become fully depleted. High sensitivity is thus achieved using thin film channels and/or low doping, as well as back-biasing the device close to depletion.

As a further example of the capabilities of the proposed approach, we have considered a 3D structure, reported in Fig. 5.

Once again, we embrace the assumption of full coverage, i.e. we describe the receptors and the target molecules as uniform dielectric layers with a dielectric constant of $2.5\varepsilon_0$, thickness 1 nm and separation Δz. Differently from the previous example, here both the target molecule layer and the receptor layer are charged and the charge is uniform across the layers. This is the case, for example, of DNA target molecules immobilized to DNA receptors. The change of conductance ΔG is defined as the difference in the conductance with target and receptor molecules (G) with respect to the case with only the receptors (G_0).

Simulation results for a device with 2 μm × 50 nm sensitive top gate area are reported in Fig. 6 considering a charge density of target molecules and receptors (assumed to be equal) of 1.5×10^{11} cm^{-2}, which roughly corresponds to 20 DNA molecules (10 receptors + 10 target molecules) per device. Since the molecule charge is negative, it further depletes the channel with respect to the depletion caused by the receptors, thus the conductance is reduced. The sensitivity increases at low V_{BG} because the channel is closer to depletion. The figure also shows the effect of the distance Δz between the target molecules and the receptors for different molar concentration. For $\Delta z = 0$ the molar concentration of the ions in the electrolyte has a minor effect on the variation of the conductance. However, for $\Delta z = 5$ nm the sensitivity becomes essentially zero in the case of high ion concentration. In fact, whereas for $c_0 = 1.5$ mM the Debye length in the electrolyte is $\lambda_{el} = 8$ nm and thus comparable with Δz, for $c_0 = 150$ mM we have $\lambda_{el} = 0.8$ nm.

4. Double layer modeling in nano-electrodes biosensors

As already mentioned, the proposed approach does not model volume exclusion and steric effects due to the finite size of the ions at the electrolyte/dielectric interface [9,14]. To investigate this aspect in more detail, we have used the full-custom simulator presented in [15] to determine reference solutions for the concentration and potential profiles of a simple one-dimensional system where one electrode is ideally polarisable and in contact with the

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[2] The dielectric permittivity is set to the most appropriate value according to salinity and temperature [18]. For the sake of simplicity, in the following, it has been taken equal to $80\varepsilon_0$.

[3] We indicate the charge per unit area because this number is more meaningful, although the charged molecules are described by a charge that is uniformly distributed over the 5 nm dielectric layer.