Simulation of 2D-material based BioFETs targeting single-molecule detection applications

Poster - Abstract ID: 196

Mr. Alejandro Toral-Lopez [1], ***Dr. Enrique Gonzalez-marín*** [1], ***Mr. Alberto Medina*** [1], ***Prof. Francisco Ruiz*** [1], ***Prof. Noel Rodriguez*** [1], ***Prof. Andrés Godoy*** [1]

1. *University of Granada*

Introduction

2D-materials based BioFETs show up as a promising alternative to nanowire based BioFETs, thanks to their higher sensitivity, compatibility with planar technology and easier surface functionalization [1]. Additionally, this technology facilitates the possibility to fully integrate signal processing stages with the sensor.

Methods

BioFETs are simulated as described in [2]. The electrostatic semiconductor-electrolyte coupling is evaluated by solving the 2D Poisson equation. The net charge is defined by the semiconductor carrier density and the electrolyte ion concentrations. The former is calculated using a 1D Drift-Diffusion transport model. For the latter, a 0.01M Phosphate-Buffered Saline is considered, with the target molecules corresponding to DNA chains of 120 pairs, modelled as solid boxes for the ion distribution [2]. The dependence of the semiconductor carrier mobility on the electric field is also considered.

Results

Three devices are evaluated (Fig.-1b, c and d) sharing the general structure depicted in Fig.-1a. Fig.-2a shows the I_{DS}-V_{FG} curve and sensor output of the first device varying the number of molecules (N_M) from 0 to 5. As it is shown, increasing N_M reduces the current of the device, but for N_M>3, the I_{DS} reduction saturates. In order to relate this saturation with the spatial density of molecules in the receptor layer, a longer device is simulated obtaining the I-V depicted in Fig.-2b. In this case, the saturation of the sensor output with N_M is clearly reduced. Therefore, we can control the saturation of the response by controlling the density of molecules in the receptor layer. Following this argument, and aiming to obtain a single molecule sensor, we test a structure with a trench in the top oxide where the receptor layer is located. As shown in Fig.-2c, when the trench is used, the I-N_M saturation is achieved for N_M>1, i.e. there are only three output states:N_M=0,N_M=1,N_M>1, being possible to clearly distinguish the N_M=1 and N_M>1 scenarios.

Discussion

We demonstrate via detailed numerical simulation how single-molecule 2D-based BioFETs behave in a complex electrolyte environment, and we analyse how the topology of the top oxide can be used to control the sensor behaviour.

[1] DOI:10.1039/c6cs00827e

[2] DOI:10.1039/c8na00109j