Models for Simulation Based Selection of 3D Multilayered Graphene Biosensors

E.Lacatus[1], G.C. Alecu[1], A. Tudor[1]

[1]Politehnica University of Bucharest, București, Romania

Abstract

INTRODUCTION:
At the forefront of a new generation of sensors graphene based devices are intensively studied for medical and bio-sensing applications.
With large similarities to the surface of graphite (Figure 1), graphene (G) can adsorb and desorb different type of atoms and molecules, remaining highly conductive [1]. This property can be used for sensor applications.
It is largely known that single- layer graphene (1G) is much more reactive than 2G, 3G (<10 layers) graphene multilayer structures [2,3]. However, the edge of the graphene is more reactive than the surface, graphene being a fairly inert material, and thus an ideal candidate for bio-sensors.
The aim of the modeling and simulation of the multilayered graphene structures is mainly focused on the device response at different types of energy stimulus reaching the active surfaces of the 3D bio-sensing structures under the main restrictions of bio-compatibility and non-toxicity (Figure 2, Figure 3).

USE OF COMSOL MULTIPHYSICS®:
For the envisaged multilayer graphene bio-sensing device structures a graphene model was firstly created in ChemBio 3D Ultra®. Its characteristics have been exported to MATLAB®, and thus different process parameters and material properties were consistently interlinked for further analyses and simulations.
The MATLAB® model and the associated properties were exported through the LiveLink™ for MATLAB® add-on in COMSOL Multiphysics® and thus the variability of the structure properties (Figure 3) could be properly analyzed in at the device scale (Figure 3,4).

RESULTS:
A large number of device module types have been tested in order to define the best response for the polymer layer between the graphene sheets. For each of these the biologic responses and the field excitations have to reach simultaneity under the COMSOL model (Figure 4)

CONCLUSION:
Making the best use of the flexible modules of COMSOL Multiphysics® of the most relevant device properties of the multilayered graphene biocompatible structures could be determined and mostly important, could be related to the complex interface phenomena at human skin level.

Reference

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Figures used in the abstract

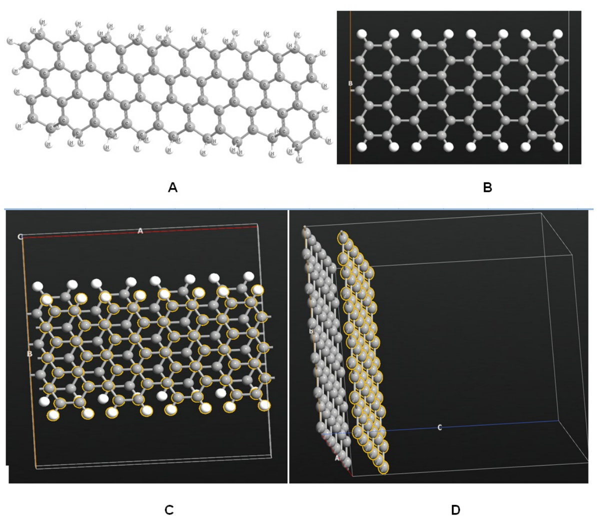

Figure 1: ChemBio 3D Ultra ® 1G -armchair structure (A) exported to Virtual NanoLab-Atomistix ToolKit® and MATLAB ® (B); 2 G – Zigzag Armchair (AB) configuration (C, D)

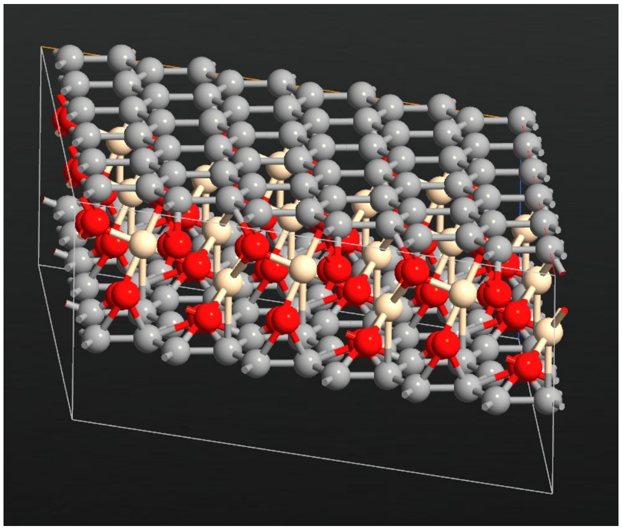

Figure 2: Multilayer 2G –Polymer- silicon glass structure exported in MATCAD ® and thereafter through LiveLink™ for MATLAB® add-on in COMSOL Multiphysics®

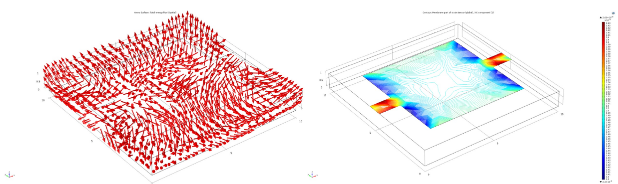

Figure 3: COMSOL Multiphysics® model of 2G biosensor Energy Flux and 2G strain tensor

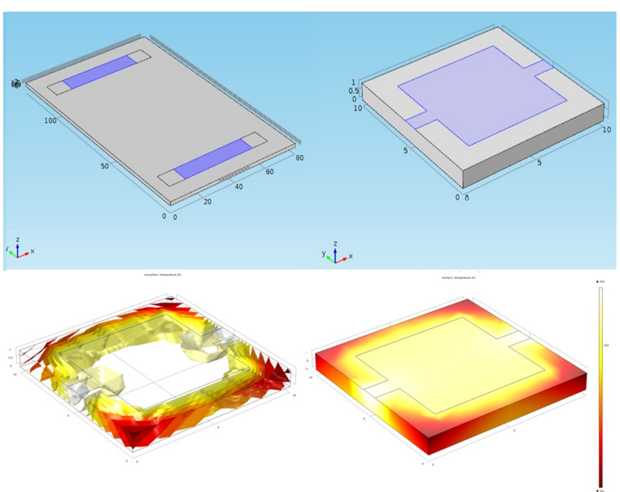

Figure 4: COMSOL Multiphysics® 2G-SiO2-Polymer device design and thermal stress simulation (Ag electrodes on silicon glass; 2G-Polymer sandwich structure on silicon glass)