COMSOL Multiphysics Simulation of Functionalized 3D Biocompatible Porous Graphene Composites

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1. Introduction

Graphene is an allotrope of carbon having the structure of a plane sp^2-hybridized atom with a band length of 1.42Å, and representing the basis of any carbonaceous material. This 2D material consisting on pure forms of carbon exhibits high crystalline and electronic quality. Thus, despite being alike an indefinitely large aromatic molecule, graphene has exceptional mechanical, electrical and thermal properties. Furthermore, being one-layer thick is almost transparent, thus interacting with light and with other materials in unprecedented ways within functionalized graphene embedded composites (fig.1,2)

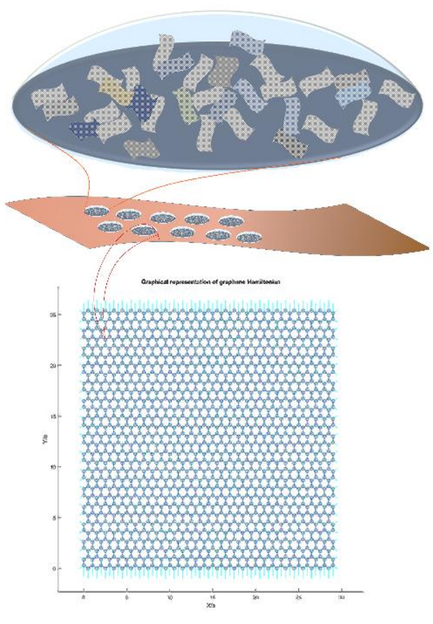

Figure 1. Biosensing device model with graphene composite cells on biocompatible porous substrate

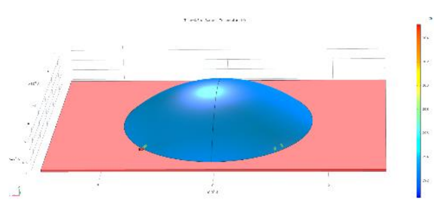

Figure 2. Individual composite (G/GO) embedded cell

2. Experimental Set-up

G/GO related physics was introduced in COMSOL Multiphysics through the bidirectional interface with MATLAB® via LiveLink™ for MATLAB.

As well, Schrödinger Equations from Semiconductors module of COMSOL Multiphysics® was used for the very particular properties of G/GO structures. But, the geometry of G/GO and of the biosensor parts were exported as SolidWorks® models through LiveLink™ for SolidWorks® add-on in COMSOL Multiphysics®

3. Use of Simulation Apps

The biosensing unit cell was designed as a multi-layered structure, each layer geometry being designed using SolidWorks. The electrical and thermal properties of plane and wrinkled/twisted G/GO structures were determined in MATLAB using SoA related data from literature and from previous studies [1,2,,3,4]

Different biocompatible layers and G/GO functionalized composite structures were modelled, designed and simulated as packed-on cells on flexible support.

Beyond the amazing theoretical properties of G sheets, the effective application of these carbonaceous material has to face a lot of technological challenges. Obviously, usual scaling-up techniques are not suitable for this class of materials due to their properties' lack of stability under normal environmental conditions.

For a proper use of their exceptional potential, these G/GO individual structures should be embedded in other material support. These host materials are limiting the extends of some properties, but would make the G/GO functionalized structures more stable, predictable and reliable.

4. Simulation Results

Thus, for these (G/GO) wrinkled/twisted (normal od porous) structures the MATLAB determined material properties and Solid Works geometrical parts and assemblies' configurations were exported in

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COMSOL Multiphysics®.Here, the MATLAB determined material properties for G/GO were added to Material Library dBs. The use of COMSOL Multiphysics® was mainly focused on heat transfer modules (shells, films, porous media, bioheat) but Schrödinger Equations from Semiconductors Module was used as well, for the very particular properties of G/GO structures.

Having successive porous, semiconductor, G/GO composite layers and shells the thermal studies envisaged these packed structures heating rate under biological and environmental (natural or focused) stimuli.

Different mesh structures were assigned for studies considering individual composite cells (fig.1) or G/GO functionalized composite layers (fig.5)

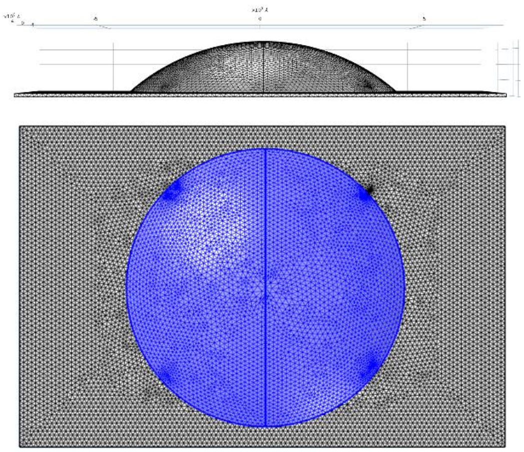

Figure 3. Mesh of graphene embedded structures

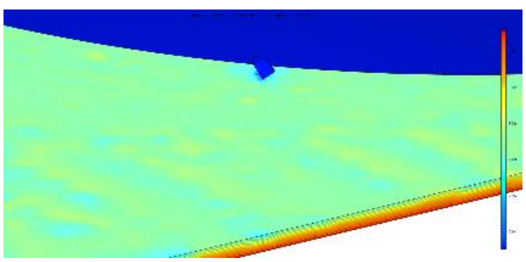

Figure 4. Physical model of biocompatible (G/GO) composite cell

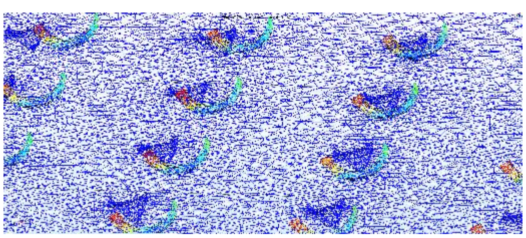

Figure 5. Mesh of graphene embedded structures

As well, the heating rate was studied on individual layers (fig.5, 6) and on assembly structures (fig.7-16).

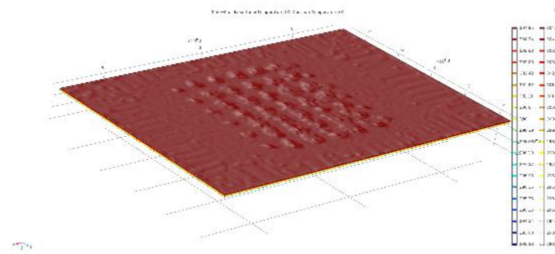

Figure 6. Thermal response of the biosensor substrate (reverse side)

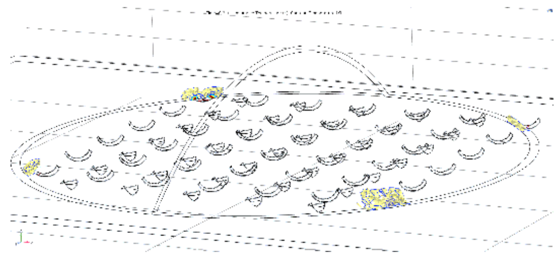

Figure 7. Encapsulated individual cell - (G/GO) singularities on shields

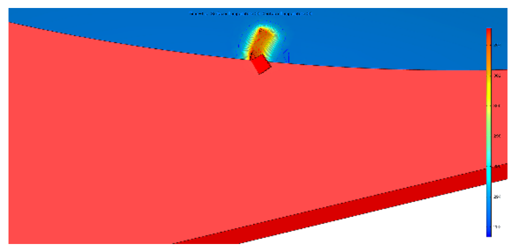

Figure 8. Thermal excitation of encapsulated individual cell (G/GO) biocompatible composite device

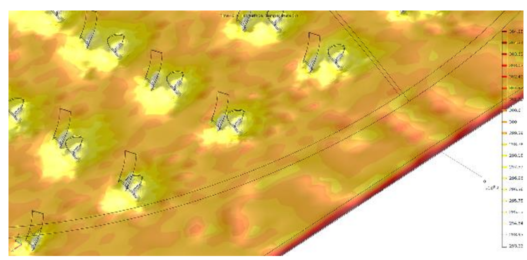

Figure 9. Successive layers and shells containing (G/GO) structures

Different G/GO geometries and composite embedding positions were analyzed.

(G/GO) response rate has been reported to the composite support and to the porous biocompatible substrate heating response on these preliminary studies.In process-data from photodermal therapy (PTT) and photodynamic therapy (PDT) were used to excite the individual unit cells through the transparent shield structure

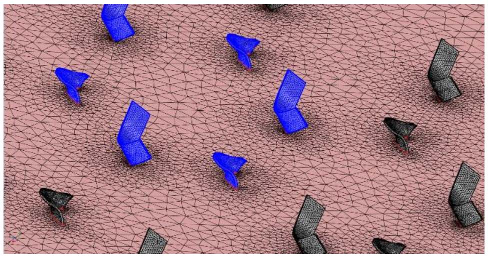

Figure 10. Mesh of the excited G/GO – composite (array)

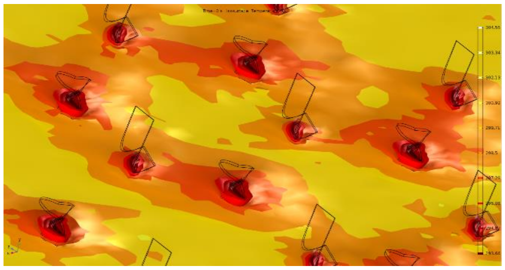

Figure 11. Response of the excited G/GO – composite (global effect)

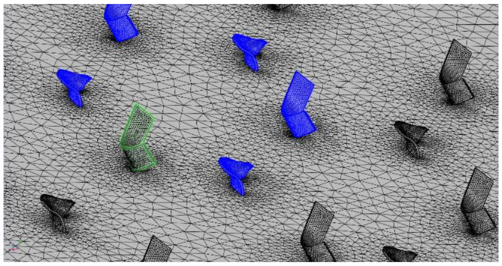

Figure 12. Mesh of the excited G/GO – composite (individual)

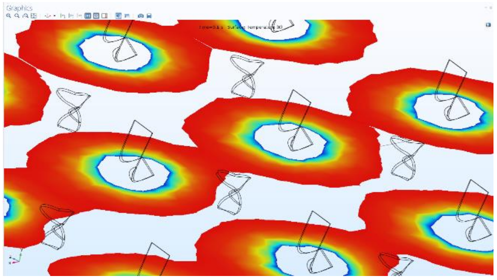

Figure 13. Response of the excited G/GO – composite (singularities chain)

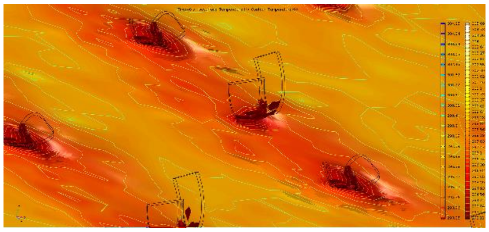

Figure 14. Time differentiated thermal response of excited G/GO structures to simulation data (t_0- skin contact)

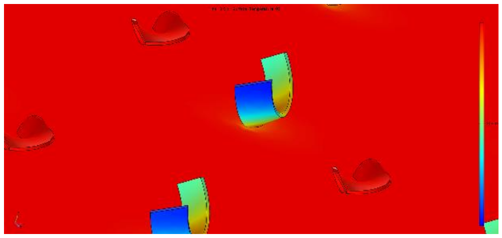

Figure 15. Time differentiated thermal response of excited G/GO structures to simulation data [(t_0 + 5s) – biosensor calibration time]

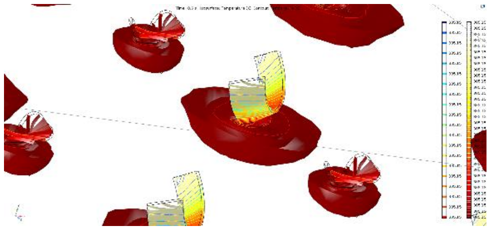

Figure 16. Time differentiated thermal response of excited G/GO structures to simulation data [$t_0 < t < (t_0 + 5s)$] –transitory response-G/G0 activation]

5. Conclusions

The results of the COMSOL Multiphysics simulations for functionalized 3D biocompatible porous G/GO composites were validated using SoA literature data related to photodermal therapy (PTT), photodynamic therapy (PDT) and drug delivery through skin processes and parameters.

These preliminary studies demonstrate the influence of the G/GO shape, size and position on the functionalized composites. These data, related to quality and stability ones, would made affordable and reliable graphene biosensors on future, making the best use of modelling and simulation complex tools.

References

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