

# A model to explain local anodic oxidation of graphene from fundamental physical principles

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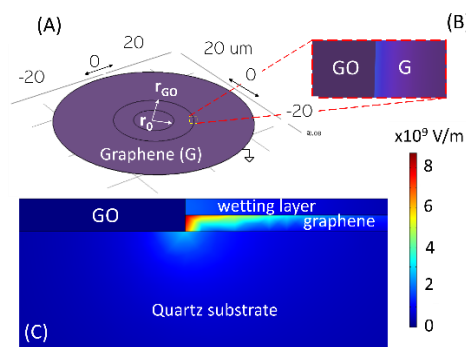
## Abstract

Oxides of graphene and other 2D materials are more reactive than those of conventional metals due to their exposed polar functional groups. This property makes them ideal for immobilizing bioreceptors on these reactive groups, which is the first step to manufacture biosensor platforms. In 2019, the authors demonstrated the ability to scale up the local anodic oxidation of graphene for industrial applications. Working at speeds  $10^4$  times faster and over sizes  $10^7$  times larger than the current records by conventional nano-probes, we were able to obtain graphene oxide spots with radius of up to 100  $\mu\text{m}$ , in less than 100 ms. [1] These spots can be added to create any desired pattern at a mm scale in just minutes. At this scale, the paradigm on the creation of a water meniscus just below the probe to explain the local oxidation is no longer operative. We propose a new model to explain how the oxidized spot radius expands over time using Boltzmann statistics and physical magnitudes (energetic barrier for incorporation of oxyanions, and its dependency on radius and applied voltage). As a result, a function  $t(r)$  describing inversely the spot radius ( $r$ ) expansion along time ( $t$ ), is obtained. The unknown energetic barrier for incorporation of oxyanions, and its dependency on radius, may be determined by fitting the model to experimental data including our own data (in case of graphene) [1], and data from other works in the literature (in case of TMDCG) [2]. In addition, we have developed a simple electrostatic model for a multilayer stack that includes the semiconductor properties of the 2D layer to be oxidized. Through finite element calculations, we solve the Poisson equation self-consistently and obtain electrical magnitudes, such as electric field (Fig. 1), and the potential drop from the wetting layer to the active material near the edge of the oxidized region. This potential decrease aligns with the potential barriers obtained from fitting the experimental curve, confirming the predictive nature of our model.

## References

- [1] S. J. Quesada, F. Borrás, M. García-Vélez, C. Coya, E. Climent, C. Munuera, I. Villar, V. A. de la Peña O'Shea, A. de Andrés, A. L. Alvarez, *Small*, 15 (2019), 1902817.
- [2] B. R. Borodin, F. A. Benimetskiy, P. A. Alekseev, *Nanotechnology*, 32 (2021) 155304.

## Figures



**Figure 1:** Multilayer test structure where the value of the electric field norm is represented for probe biased at -30V. A) Cylindrical thin film stack, where  $r_0$  is tip radius, and  $r_{GO}$  that of the circular oxidized zone. B) Zoom at the frontier GO/G where the color change reveals the presence of an electric field in graphene resulting from the induced polarization charge. C) Cross section where the rebound of field intensity in graphene is observed near the GO/G boundary.