First Principles Formulation of the Local Functionalization over Time in Two-Dimensional Materials

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Abstract

Electric field-assisted covalent functionalization of graphene and other two-dimensional (2D) materials provides robustness and positional control, two crucial features when activating biosensor platforms. In particular, local anodic oxidation was proven on graphene at the nanoscale since 2008. However, it was not until 2019 that it was demonstrated to have massive application potential, scaling up to hundreds of μm^2 in less than one second. [1] These are sizes required by typical commercial biosensors based on field-effect transistors. Thus, a suitable formulation of the oxidation expansion over time is relevant to control and predict the oxidized spot size on the active biosensor regions. For that purpose, the incorporation of oxyanions at the edge of the oxidized zone has been formulated by applying Boltzmann statistics, what includes physical magnitudes such as the energetic barrier and its dependency on radius and applied voltage. As a result, a function t(r) describing inversely the increase of the spot radius (r) along time (t), is provided. The unknown energetic barrier for incorporation of oxyanions, and its dependency on radius, may be determined by fitting the model to the available experimental data. On the other hand, a simple multilayer stack including the relevant components (oxidized and 2D semiconductor layers, substrate and metallic contacts) is proposed, where 2D materials are considered as thin films. Under this approach, the Poisson equation has been solved self-consistently by finite element calculations, to obtain electrical magnitudes such as electric field throughout the structure, 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 barrier reduction along the spot radius obtained from fitting the experimental curves, confirming the predictive nature of this model either for graphene or alternative 2D Materials. [1] S. J. Quesada et al., Small, 15 (2019), 1902817.

Biography: A.L. Álvarez is full Professor of Electronics at Universidad Rey Juan Carlos, with more than 30 years of experience in Solid State Electronics. In the last 10 years, author of 22 publications in JCR (>300 citations between 2014-23, and two covers in high impact journals: Small, 40 (2019), and J. Phys. Chem Lett., 6, 11 (2020). Co-inventor of 5 patents (3 international extension), two best business ideas award, member of the European Organic Electronics Observatory (2010-2013), Spanish Electron Devices Conference Committee since 2008, and IEEE EDS since 2002. Signatory researcher in 24 competitive projects (6 European), and 8 as PI.