Streetching a defective graphene layer

César González
Manuel Lozano
Dpto Física de Materiales, Universidad Complutense de Madrid. Pza. Ciencias, s/n E-28040 Madrid, Spain
Instituto de Magnetismo Aplicado UCM-ADIF, V. Servicio A-6, 900, E-28232 Las Rozas, Spain
cesar.gonzaez@ucm.es

Abstract: Since the experimental synthesis of graphene [1], a great number of alternative two dimentional (2D) materials have been found, presenting many different properties. From the very beginning, the graphene monolayers received a great attention due to their promising conductive conditions [2] as well as their interesting chemical and mechanical properties [3]. In the recent years, the elasticity of a single graphene monolayer has been extensively studied by both experimental measurements [4] and theoretical calculations [5]. In this work, we have revisited the streetching process of a single graphene monolayer by the use of theoretical calculations based on the Density Functional Theory (DFT) as implemented in the FIREBALL code [6]. Creating a long enough unit cell of 240 atoms and implementing periodic conditions, we have found the most stable structures after moving the last 24 atoms at each side in small steps of 0.2 Å. In such process, these atoms remain fixed in the unit cell, which size have been increased accordingly in the corresponding direction. During the streetching process, we have studied the elastic and the electronic properties of the material and at the breaking point, we have found some interesting structures as the one presented in Figure 1. We have followed the same procedure with the ideal graphene as well as with some selected defects of our choice: a vacancy, a divacancy or a contaminating element (B and N). Our results allows to define the electronic change in the Dirac point with the stress introduced and the change on the elastic properties with the inclusion of the different defects. Additionally, the structures found at the end of our simulations (see Figure 1) path the way to a future thorouhg analysis of the chemical reactivity enhancement in the streetched graphene.

References

[1] Novoselov K S, Geim A K, et al, Science 306 (2004) 666.
[2] Castro Neto, A H, et al. Rev. Mod. Phys., 81 (2009) 109.
[3] Yan, L, et al. Chem. Soc. Rev., 41 (2012) 97
[4] López-Polin, G, et al. Carbon 124 (2017) 42
[5] Silva-Guillén, J A, Guinea, F, Phys. Rev. B 101 (2020) 060102(R)
[6] Lewis, J P, et al, Phys. Status Solidi B 248 (2011) 1989

Figures

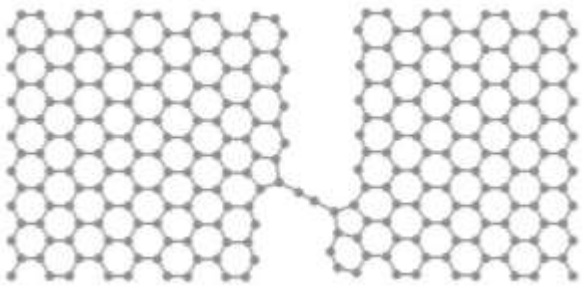

Figure 1: Final step after the streetching process of a graphene layer, resulting the formation of a atomic chain.