Simulation of the energy loss of proton beams interacting with few layer graphene foils

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Synopsis We have simulated the passage of proton beams, having energies $E < 10$ keV, through graphene targets, considering the case of few layer foils. For this purpose and for comparison, we implement Monte Carlo and deterministic semi-classical approaches to describe the interaction of protons with carbon atoms in graphene structures. Our results show that the energy loss through a single layer graphene foil is smaller than recent *ab initio* calculations based on time dependent density functional theory (TD-DFT). Besides, for $E > 6$ keV the energy loss into a graphene target composed of n layers is n times the energy loss through a single layer graphene foil.

The interaction of proton beams, having velocities $v < 1$ au ($E < 25$ keV), with graphene targets has been the subject of recent research [1-3]. In all these studies, the energy loss ΔE into a single layer of graphene practically follows a linear dependence with the projectile velocity v, although slight differences in the absolute value of ΔE appear for each calculation.

In this work, we obtain the energy loss by simulating the passage of protons through multilayered graphene targets ($n<10$ layers). For that purpose, we simulate particle trajectories inside the solid to obtain information on the energy losses parameters. Newton equations of motion of the particle under the influence of the forces due to the target nuclei and core electrons are solved assuming a screened type interaction potential. Furthermore, a quantum dissipative force resulting in an energy loss due to the electron-hole excitations of valence electrons is included using a non-linear model based on density functional formalism [4].

We show in figure 1 the calculated energy loss of a proton beam through a single layer graphene foil. It can be seen than in all cases the energy loss practically follows a linear dependence with the projectile velocity, except at the lowest velocities. However, our values for ΔE are clearly smaller than the ones obtained by methods based in TD-DFT [1-3].
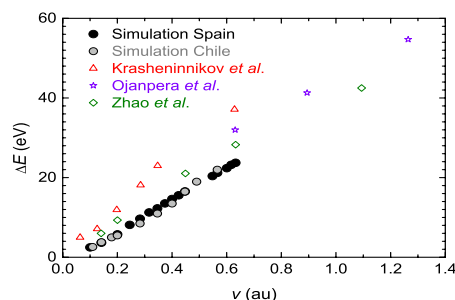
Figure 1. Energy loss of a proton beam through a single layer of graphene.

We have also simulated the passage of protons through graphene foils made of several layers. These results, presented in figure 2, clearly show that ΔE is proportional to the number of layers, for $v > 0.5$ au (i.e., $E > 6$ keV).
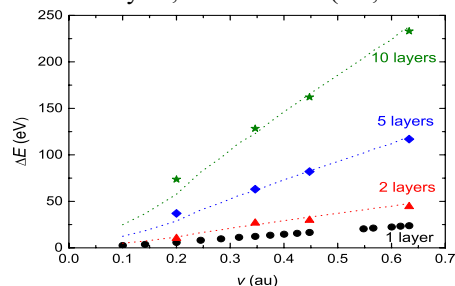
Figure 2. Energy loss of a proton beam through a few layers graphene foil: simulations (symbols) and $n \times \Delta E$ of a single layer (lines).

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References

[1] A. V. Krasheninnikov *et al*. 2007 *Phys. Rev. Lett.* **99** 016104
[2] A. Ojanperä *et al*. 2014 *Phys. Rev. B* **89** 035120
[3] S. Zhao *et al*. 2015 *J. Phys.: Condens. Matter* **27** 025401
[4] J. E. Valdés *et al*. 2013 *Carbon* **52** 137