Early electron dynamics in graphene after Swift Heavy Ion impacts

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Swift Heavy Ions could be employed to fabricate sensors and nanofilters of superb performance [1,2] out of graphene. Recent work suggested that SHIs can produce pore-like defects in suspended graphene [3]. After a SHI impact, the electrons in the material are strongly excited and an electron cascade is generated; in two-dimensional materials this process is particularly important, since the electrons can be emitted out of the layer.

In this work we investigate the initial dynamics after the ion impact in a 2D material as graphene and their role in the mechanism of defect formation. For that we employ a multiscale model which uses Monte Carlo (MC) and Time Dependent Density Functional Theory (TDDFT) to simulate the initial electronic dynamics, together with the Two-temperature Molecular Dynamics model (TTMD) to simulate the formation of defects at atomic level.

Our simulations show strong electron emission in graphene as the electron cascades develop. We observe an almost linear relation between the number of emitted electrons and the stopping power. Both techniques used MC and TDDFT show almost identical secondary electron emission spectra. In addition, TDDFT results also exhibits strong electron capture at low ion velocities. We observe with both approaches large transient positive charge in the layer around the ion impact point. The TDDFT simulations show a fast charge neutralization in graphene, similar as it was observed previously in Highly Charged Ions simulations [4]. TTMD shows a strong reduction of the nanopore size with the increase of the electron emission. These results suggest that the early electron dynamics after the SHI impact can play a decisive role in the mechanism of defect formation in 2D materials, and therefore, they should be taken into account when modelling them.

References:

[1] Han, Tae Hee, et al. "Steam etched porous graphene oxide network for chemical sensing." Journal of the American Chemical Society 133.39 (2011): 15264-15267.
[2] Jiang, De-en, Valentino R. Cooper, and Sheng Dai. "Porous graphene as the ultimate membrane for gas separation." Nano letters 9.12 (2009): 4019-4024.
[3] Vázquez, H., et al. "Creating nanoporous graphene with swift heavy ions." Carbon 114 (2017): 511-518.
[4] Gruber, Elisabeth, et al. "Ultrafast electronic response of graphene to a strong and localized electric field." Nature communications 7 (2016): 13948.