Free-standing graphene as a substrate for SIMS – molecular dynamics simulations

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Abstract

Secondary Ion Mass Spectrometry (SIMS) is a popular analytical technique providing valuable information in various fields of science and technology. Much effort is being put into improving its precision and efficiency. For example, in recent years, cluster ion beams have attracted attention due to their capacity to enhance the ejection of large intact organic molecules. [1] There are also reports on using graphene overlayer to stimulate higher signals from the investigated materials. [2] Moreover, a novel SIMS configuration, using transmission orientation, has been proposed recently. [3]
We have decided to merge the three methods and investigate cluster bombardment on free-standing graphene in transmission geometry. In our work, we used molecular dynamics computer simulations to model samples consisting of single- and many-layered graphene with and without a monolayer of phenylalanine molecules deposited on it. We bombarded the samples with a C_{60} and Ar_n cluster projectiles with an energy ranging from 0.5 to 50 keV. The investigation provides evidence on processes of emission that are unique to the graphene substrate. Firstly, the graphene layer does not have enough atoms for the traditional models to be applied. Secondly, graphene can exhibit an unusually high rate of deformation and energy absorption. Thirdly, there is a certain trampolining action, including separation of organic layer from graphene membrane, that promotes gentle emission from graphene. I will discuss all of the mentioned phenomena and give prospects of using free-standing graphene as a novel substrate for ion bombardment techniques.

References

[1] N. Winograd, The Development of Secondary Ion Mass Spectrometry (SIMS) for Imaging in The Encyclopedia of Mass Spectrometry (Elsevier, 2016)
[2] P. Michałowski et al., Scientific Reports, 7 (2017) 7479
[3] S.V. Verkhoturov et al., Journal of Chemical Physics, 150 (2019) 160901

Figures

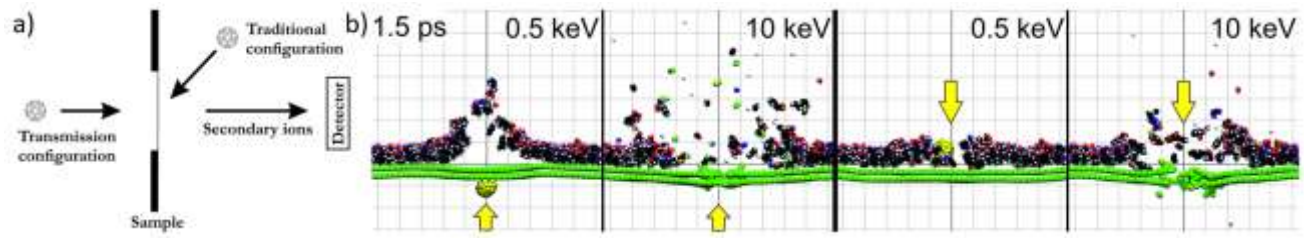

Figure 1: a) Traditional and transmission configuration of the SIMS technique. b) Simulation snapshots of bombardment with C_{60} projectile with energies of 0.5 and 10 keV into phenylalanine monolayer on graphene sample showing different impact results. Graphene atoms are green, organic atoms are a mix of darker colours, projectile atoms are yellow, yellow arrow depicts the direction of impact.