Interferences and imaging in ion impact on 2D materials

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Synopsis We present the extension of a semiclassical coupled channel approach developed in ion-atom collisions to the description of the electronic processes occurring in the course of the collisions between ions and 2D materials. By taking into account the weakly bound electrons of the material and the multi-center periodic features of the target, we are able to compute coherent differential quantities related to electronic processes induced by low charged projectiles. We illustrate the method by the description of electron transfer in keV-proton collisions on graphene single sheet and show the principles of a new imagery technics based on the measurements of differential cross sections.

Two-dimensional materials, e.g. graphene, designed with spectacular properties, possess an important potential for applications. Aside their macroscopic features, the present possibility to suspend them on boundaries opens rather new lines of studies based on their quantum properties at the atomic level. The dynamics response of graphene to strong and ultrafast perturbations is one of these lines and is still largely unexplored nowadays. For low-energy ion-impact a recent investigation [1] simulated images of graphene using the ionization process induced by 30-keV H⁺ impact on single suspended sheet. Based on time-dependent density functional theory a large part of the ultrafast electronic dynamics during the scattering event was ignored.

In that context we have developed an original method [2] to overcome the inherent difficulty to describe in a time-dependent scheme the coherent build up of probability amplitudes related to a given process from the multiple centers of the target. During the workshop we shall present this method based on state-of-the-art semiclassical non-perturbative treatment originally developed in ion-atom scattering theory: it is based on the solution of the time-dependent Schrödinger equation using scattering wavefunctions developed onto (i) the atomic orbitals centered on each site of the material and which contribute to the description of the highest occupied molecular orbital and (ii) the projectile states which mainly contribute to the transfer processes. On these latters we include electron translational factors to have Galilean invariance of the results. By close coupling scheme we can extract probabilities for a given process as function of the impact point of the projectile on the target plane (perpendicular to the projectile trajectories), see Figure 1.

We shall illustrate this approach by the modeling of the capture processes in collision between H⁺ and graphene in the low intermediate energy domain. The selectivity of the process in term of target geometry and site composition will be presented as function of impact velocity (Figure 1). A simple and illuminating model will be presented in order to explain the coherent multicenter effects giving rise to a surprising contrasted image of the material for a specific velocity. This behavior opens the way to the principles of a new imagery technique for periodic two-dimensional materials.

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Figure 1. Total capture probability distribution in an asymptotic plane parallel to the graphene sheet. Two energies (left panel: 1keV - right panel: 7.5 keV) are considered for H⁺ projectiles impacting perpendicularly the target plane (drawn from [2])

References


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