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Perforation of 2D-structures by impact of highly charged ions

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In the past two decades it has become possible to isolate monolayers of bulk materials. These new types of target materials are effectively 2-dimensional (2D) and as such have opened up new possibilities for material research. In particular, we are interested in the response of these targets to strong fields when irradiated with highly charged ions (HCI) often leading to pore formation in the layer. A complete description of the interaction of HCIs impinging on 2D materials is clearly out of reach as the interaction is governed by multi-particle processes such as the polarization of the layer ensuing the acceleration of the HCI by the 2D equivalent of its image charge, the charge transfer dynamics between HCI and the 2D material at smaller distances, the nuclear stopping upon impact on the target layer, and the neutralization dynamics of the charge depleted area left by the HCI around the impact point. To make the problem accessible we have set up a Monte-Carlo simulation combining a molecular-dynamics simulation for the target atoms with hole-hopping conduction after extraction of electrons by the impinging HCI. Depending on the conductivity of the simulated material (free parameter in simulation) we observe pore formation in qualitative agreement with experiment.
While charge transfer and surface damage after impact of HCI on solid surfaces has been investigated in detail, both of which could be well described by the classical-over-the-barrier (COB) model and classical molecular-dynamics simulations, similar interaction systems, however, are not yet well understood for 2D target materials. Due to the limited conductivity of the layer which results in a reduced total number of electrons available for charge-exchange processes for the neutralization of the HCI and, following this charge transfer to the projectile, the neutralization of the impact area are expected to proceed slower increasing the time available for Coulomb explosion.
We have combined the COB model for the electron transfer from the target layer to the HCI with a charge hopping model for charge conduction within the 2D material. These two models are integrated into a molecular-dynamics simulation for the motion of the target atoms. To model the nuclear dynamics we use a Stilling-Weber potential valid for graphene layers with a varying number of carbon rings around the impact point. Depending on the conductivity (i.e. hopping time) chosen for the simulation, different target sizes had to be used in order to achieve convergence of the numerical results.
As free parameters in the simulation we vary the initial charge state Q_{in} of the HCI as well as the hopping rate $f_h = t_h^{-1}$
(mobility) of positive hole charges. Diffusion constants (hopping rates) for different targets have been estimated from the band structure of the materials. Certainly, hopping conduction is not a suitable model for (semi-)metallic conduction as in ground-state graphene but can be used for any material with (small) band gaps as can be expected to be induced also in graphene in the Coulomb field of the approaching HCI. Other materials such as, e.g., MoS2 (large band gap) or Fluorographene

with a conductivity depending on the degree of fluorination are well described by hole hopping models.
We determine regions of stability (blue) and pore formation (pink) of the target as a function of Q_{in} and t_h (Fig. 1) with the release of a single target atom defining the limit of stability. The functional dependence of the line separating regions of stability and instability is well fitted by $Q_{in} \sim (t_h - \tau_c)^{-\frac{1}{2}}$. Qualitatively, our simulation reproduces available experimental data, i.e., we find pore formation for MoS2 (well in the pink area for all charge states) and stability for graphene (on the left border of Fig. 1). Experiments of Fluorographene layers as target and HCI with a wide range of initial charge states Qin were recently performed. To examine the transition region, comparisons to the Fluorographene experimental data will allow us to benchmark and further improve our simulation.
Future experiments exploiting the capabilities of HITRAP to provide very highly charged ions at very small kinetic energies (long interaction times) will allow to test the stability of graphene in this extreme region of interest. Based on our simulation we will be able to assess the electronic properties of graphene under extreme conditions.

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