Model for Nanopore Formation in Two-Dimensional Materials by Impact of Highly Charged Ions

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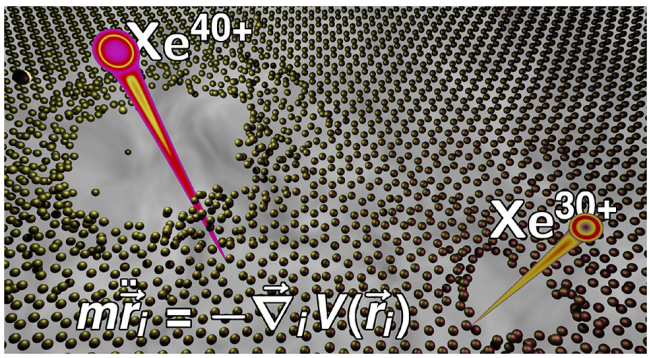

We investigate the response of 2-dimensional structures to the transmission of highly charged ions (HCIs) from the first electron transfer from the target to the projectiles locally charging up the impact area to the emission of excess electrons and target atoms leaving behind nanopores in the 2d-material thereby changing target properties. Aim of our studies is the control of nanopore formation which may lead to technical applications like, e.g., water purification or gas filtering.

It has been found that hole formation depends on both target properties, in particular its electron mobility, as well as the charge state of the incoming projectile, i.e., the potential energy carried into the collision [1]. Experiments have been conducted with multiple targets ranging from conducting single-layer graphene (SLG) to MoS_2 with an electron mobility three orders of magnitude smaller. While the high electron mobility in SLG enables fast reneutralization of the electron-depleted impact area thus ensuring long-time stability of the target, MoS_2 may disintegrate when excited by an HCI due to the formation of a long-lasting charge patch initiating Coulomb-driven disintegration of the target layer. It was found that a minimum charge state Q_{in} of the projectile was required in order to produce nanopores [2].

To investigate the hypothesis of Coulomb-driven hole formation, we have recently set up a simulation modeling all three aspects of the process, the electron transfer to the projectile, charge transport in the target, and a molecular-dynamics simulation for the motion of atoms in the 2d-structure in the presence of Coulomb forces [3].

Based on the charge mobility of 2D materials, this model is able to reproduce the dependence of the pore diameter on the initial charge state of the impinging projectile or the reduction of the number of electrons extracted from materials with small charge mobility. Only for single-layer graphene, a material with high mobility, pore formation was not observed irrespective of the incident charge Q_{in}. For other materials characterized by their conductivity we find a

threshold charge for pore formation that approximately depends on the square root of the charge mobility.

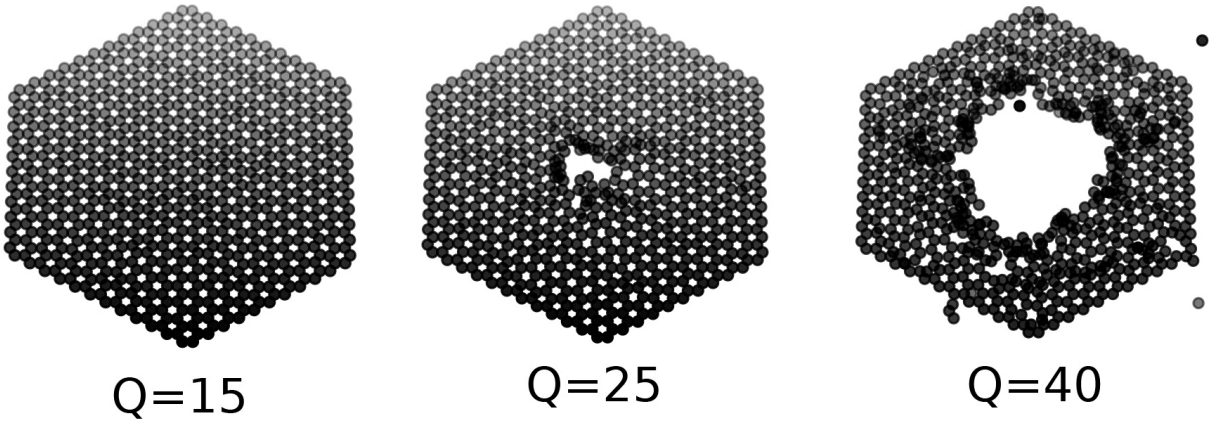

Fig. 1: Dependence of hole diameter on the charge state of the incident ion. For materials with a conductivity larger than that of graphene a threshold behavior has been observed in the simulation which qualitatively reproduces the results of experiments performed so far.$

The stability of a target material irradiated by HCIs can be represented in phase diagram as a function of the initial charge state of the projectile and the relevant material parameter of the 2D structure, its charge mobility. Based on comparisons of our simulation results with experimental data we expect that our predictions should properly capture the qualitative dependences of pore formation in HCI–2D layer interactions.

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