Development of an advanced water filtering system based on graphene irradiated by gas cluster and highly charged ions

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Effects of a heavy low energy ion bombardment of various materials are explored for the purposes of creating new materials that have advanced properties. In this study, features of the defects' formation in the samples of graphene, graphene oxide and silicon by Ar cluster ions irradiation are given. Irradiation was performed by Ar cluster ions with acceleration energy 30 kV and total fluence of Ar cluster ions ranged from $1x10^9$ cm^{-2} to $1x10^{13}$ cm^{-2}. Samples of multi-layer graphene oxide, mono-(SLG), few-layer (FLW) of graphene and polished Si are used for irradiation experiments. Characterization of the irradiated samples was conducted by the methods of Raman spectroscopy, atomic force microscopy and NEXAFS. Irradiation of graphene, graphene oxide and silicon resulted in crater/defect formation over the surface. Small pores on the surface of the graphene oxide samples were formed under such parameters, with the mean pore size of 10-20 nm and depth of 2-4 nm. AFM results proved the presence of nanopores on graphene oxide structure. AFM images of irradiated silicon shows formation of craters on surface of silicon with crater dimension of 20 nm in diameter and 1 nm deep. The distribution of craters was concordant with the Gaussian distribution of the mass-to-charge ratio for individual clusters measured using TOF and the size distribution with an average size of aout 1000 atoms per cluster. Additionally to AFM irradiated samples of graphene, graphene oxide and silicon was characterized by Raman spectroscopy. Characteristics of the defects formation in the samples of graphene oxide produced by cluster ions were compared to those by highly charged $_{131}Xe^{+22}$ ions, with flunces of 10^{12}-10^{15} ions/cm^2 and with kinetic energy 1.75 MeV were presented. The analysis of irradiated samples was conducted by using Raman spectroscopy and the near edge X-ray absorption fine structure (NEXAFS). Computer simulations of defects were studied by multiscale method. Ab-initio DFT was applied to study mono- and divacancies in momolayer and multilayer graphene. Individual gas cluster ion impacts on suspended graphene sheet and a graphene on vadious substrates were carried out using Sandia Labs Lammps package and the results were passed to a finite element Comsol multiphysics package for the development of a porous media filtering system.