Surface modification of graphene by GCIB

Ion irradiation by gas cluster ion beams (GCIB) has been used for introducing defects into graphene sheets on SiO2, in bulk MoS2 and in multilayer graphene oxide in the form of nanopores. Atomic force microscopy (AFM) and Raman spectroscopy were utilized to conduct characterization and investigation of disorder formation in structure of irradiated samples of graphene on SiO2, bulk MoS2 and multilayer graphene oxide. Uniformly distributed craters and defects on the surfaces of graphene, graphene oxide and bulk MoS2 by cluster beams were observed after GCIB irradiation. AFM showed formation of nanopores in graphene, graphene oxide and bulk MoS2 upon irradiation by Ar clusters with 30 keV and with fluence in the range $10^9$-10$^{13}$. Raman spectroscopy of irradiated samples of graphene with different amount layers has demonstrated the growth of D peak which indicates amount of disorder in graphene structure. Ab-initio density-functional theory (DFT) was used to study point defects and a large scale parallel molecular-dynamics (MD) simulations were used for studying formation of gas cluster ion impacts. The results of simulations were compared with experimental craters and surface shape.