SPUTTERING OF GRAPHENE BY HYDROGEN-CARBOn CLUSTERS: CH, CH2, CH3 and CH4

F. Umarov 1, I. Yadgarov 2, V. Stelmakh 2 , A. Ulukmuradov 2

1Kazakh-British Technical University, Almaty, Kazakhstan

2Ion-plasmous and Laser Technologies Institute after Arifov, Tashkent, Uzbekistan

Computer model of graphene of rectangular form consisting of 112 carbon atoms in the planar hexagonal packing, was built with imposition of periodic conditions on boundary atoms along the plane of the structure with a corresponding "heating" up to 300 K. Computer models of CH, CH2, CH3 and CH4 were built without imposition of periodic conditions and without the "heating". In these and subsequent simulations Brenner potential second generation (1) was used. Once the model of graphene was obtained, by computer simulation processes of sputtering of graphene at normal incidence with different energies of CH, CH2, CH3 and CH4, also carbon atoms for comparison, were studied. At first the minimum kinetic energy for sputtering of graphene at normal incidence of carbon atoms has been identified and this energy was found to be 22.5 electron-volts. Then for different values of energy and types of the hydrogen-carbon clusters 100 of incidences onto a randomly chosen point of the surface the graphene were simulated.

The minimum kinetic energies for sputtering of graphene by different types of the hydrogen-carbon clusters and changing of structure of graphene were obtained and discussed.

REFERENCE

1. D. W. Brenner, O. A. Shenderova, J. A. Harrison, S. J. Stuart, B. Ni, S. B. Sinnot // J. Phys: Condens. Matter. − 2002. − 14. − 783-802.