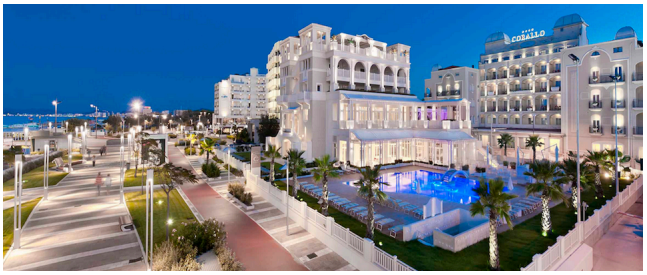

Contribution ID: **70** Type: **poster**

Ion Irradiated Aligned Multiwall Carbon Nanotubes Physical Properties

Monday, 5 June 2023 18:18 (1 minute)

The combination of chemical and physical processes is the main mechanism of the CNTs' bactericidal action. The mechanism of the antibacterial effect of nanomaterials has not been sufficiently studied to date. Changing the structure of carbon nanomaterials by ion beams allows one to adjust their electrical and magnetic properties, vary the thermal conductivity of individual carbon nanofibers, change the wettability of various liquids on the surface, increase the sensitivity to certain gases by surface defect engineering, etc.

We have recently reported that 80 keV He+ ion irradiation helps to obtain MWNT-based surfaces with tunable wettability, [1],which can be significantly varied from hydrophilic to superhydrophobic behavior, such properties have prospects in biomedical applications.

All abstracts must be written in English and occupy a maximum of 1 page A4 written in Times New Roman 12, alignment in mode "justify". Please make sure to respect the following margins: top, bottom, right: 25 mm; left: 30 mm.

Modeling the interaction of irradiated carbon nanomaterials, especially carbon nanotubes, with environmental gas molecules is often not taken into account when calculating the ionic modification of such materials.The present study is aimed at modeling the interaction of carbon nanotubes irradiated with an ion beam with environmental gas models. For the calculation under consideration, the interaction of four types of atoms in the simulated system was taken into account according to the PeahFF potential, the total number of atoms of the simulated system was about 300 thousand.The network of bonds was analyzed in order to search for defects in its structure.Simulation was done with help of Lomonosov-2 supercomputer [2] on gprahical processor unit (GPU) nodes with up to 10 times acceleration..

As a result of simulation the ion irradiation of multi-walled carbon nanotubes (MWNTs) with inert gas ions, it was shown that complex defects can form in the inner layers, including those caused by recoil atoms, dusting of inner shells, thermal annealing, and other processes caused by ion irradiation. Such defects changed the conductivity type of the nanotube, and upon functionalization, they were able to become a detecting element of a sensor built on the basis of ion-modified CNTs.

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