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Channeling of low-energy ions in carbon nanotubes taking into account many-body effects

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The use of carbon nanotube (CNT) bundles instead of masks has the advantage of allowing the ion beam to be controlled in three dimensions by manipulating the nanotubes. Due to this, it becomes possible to direct the ion beam to hard-to-reach places, for example, in the manufacture of microelectromechanical systems (MEMS) or nanoelectromechanical systems (NEMS), as well as in the creation of semiconductor devices with a complex spatial architecture. The aim of this study was to study the passage of low-energy ions through carbon nanotubes in the channeling mode. Problems that were solved: 1. The study of elastic perturbations of the CNT wall when low-energy particles are channeled into them. 2. Accounting for the effect of wall perturbations on the motion of particles in CNTs.

The method of molecular dynamics was used to solve the set problems. the LAMMPS package [1] was used, the interaction between carbon atoms in a carbon nanotube was described using the AIREBO potential [2, 3], and between an ion and carbon atoms using the Ziegler-Biersack-Littmark (ZBL) potential [4]. The deceleration on the electron gas was taken into account according to the method [5]. Calculations were made using the Lomonosov supercomputer center of Lomonosov Moscow State University. M.V. Lomonosov [6].

Using the example of Ar⁺ ions with an energy of 100 eV, it is shown that when an ion moves with angles close to critical, after its collision with a CNT wall (10, 10), wall perturbations arise - deformation waves that affect the motion of the channeled particle. The motion of the channeled particle after the first collision leads to the exchange of energy between the elastic perturbation of the wall and the channeled particle. In the case when the velocities of their longitudinal motion are close, this leads to a twofold decrease in the energy loss of the moving particle in each collision with the wall as compared to the case of motion without taking into account perturbations of the nanotube wall.

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