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PS3-14 Energy Characteristics of Particles of Atomic Flux in Carbon Nanotube

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In modern works by channeling in carbon nanotubes treated basically the process of ion [1] and the proton channeling. In our work, we have attempted to examine the process of channeling atomic flux consisting of 50 or more particles. Basic atoms that were considered is O, H, N.

In the simulation, we used LAMMPS [2] with developing interatomic potentials ReaxFF. Currently, we investigated the losses of atomic flux energy in the CNT with different geometry and with different initial energy of the atoms. An assessment of the structure of the tube after a long channeling (2-3 picoseconds). It is shown that the small part of the hydrogen atoms dechanneling through the tube. For the oxygen atoms characteristic deformation of the tube and its subsequent destruction.

References

- [1] Titus A. Beu, J. Chem. Phys., (2010) 132, 164513.
- [2] <http://lammps.sandia.gov>

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