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Mechanisms of destruction of MWCNTs of various diameters under ion irradiation

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Previously, in experiments with irradiation of multi-walled carbon nanotubes, it was shown that nanotubes with a smaller number of layers are destroyed more strongly than thicker-walled nanotubes at the same irradiation fluences with He⁺ ions [1]. In this work, the ion-induced destruction of MWCNTs was modeled using the classical molecular dynamics method using the LAMMPS code [2] and AIREBO-M potentials [3], as well as taking into account electronic braking.

The model considered 5 different MWCNT diameters. As a result of the simulation, approaches to explaining the mechanisms of different behavior of thin-walled and thick-walled nanotubes under the same irradiation conditions are discussed.

The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University [4].

References

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