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Processes of decollimation of the beam of fullerenes during scattering on it beam of hydrogen.

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Abstract content
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Fullerene with impurities inside (X@C60, where X is N, P, and etc. atoms) can be used as the unit cells for quantum computers (for example, [1]). Based on experimental work [2], and using molecular dynamics method with Brenner interatomic potential [3], we studied a penetration of 8-15 eV hydrogen (H) atoms into fullerenes beam (20 fullerenes, 1eV/molecule). This simulation can be applied to other atoms replacing the Brenner potential by the suitable interatomic potentials. One of our goals was to clarify the mechanism decollimation of beam of fullerene in scattering onto them hydrogen atoms. Process of decollimation of beam of fullerenes may be of some importance in the preparation of nanoelectronic components in this way. The simulation results show that interaction of low-energy beams of fullerenes and hydrogen atoms have pronounced inelastic character.

The transverse velocities, acquired fullerenes as a result of their interaction with hydrogen, are comparable with the velocity of deposition of fullerenes. It can lead to significant spread of fullerenes on the substrate on which they are deposited. When energy of the beam of hydrogen atoms increased, process of decollimation of fullerenes is reduced.

At carrying out of such model calculations should be careful with choice the density of the beam. When the number of atoms in the beam and its energy increase simultaneously, partial or complete destruction of fullerenes can observed.

References

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