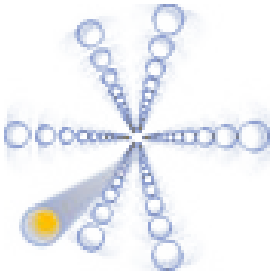

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PS3-23 Hydrogen Atoms Channeling through Carbon Nanotubes

Thursday, October 9, 2014 5:00 PM (1h 30m)

Using molecular dynamics method with Brenner interatomic potential [1], we studied the channeling of ideally collimated beam of hydrogen atoms (1000 atoms, 100-250eV/atom) through carbon nanotubes (CNT). CNT with diameter of 13.6 angstroms were placed in one plane, parallel to each other at a distance apart 3 angstroms. Hydrogen atoms are directed along the axes of the tubes. During H interaction with CNT a part of H atoms is scattered by the face of the tube, some of them (having undergone one or more collisions inside the tube) are dissipated through the wall, and other part of H atoms is channeled through tubes. We studied these channeled atoms. As results show that these atoms consist of 40-53% of the total number of H atoms.

We have analyzed the angular distributions of H atoms channeled through the tubes. These H atoms are slightly deflected from an initial direction, basically, in the range from 0 to 20 degrees. 20-25% (of total) atoms is scattered in the range from 0 to 1 degree. 20-28% (of total) atoms is scattered, mainly, in the range from 1 to 20 degrees. Distribution is continuous with main peak at 0 degree. With sequential increase of the energy of the incident beam (from 100 to 250 eV/atom), the number of hydrogen atoms channeled through the CNTs is increased, however, the range of scattering angles remained the same - 0-20 degrees.

Setting a screen at some distance (100-1000 angstroms) from the ends of the nanotubes, we got a projection of H atoms on the screen after channeling them through CNT. Diameter of these projections is 10-11 angstroms, which is slightly smaller than the diameter of nanotubes (13.6 angstroms). Diameter of these projections does not depend on the energy of beam (in 100-250eV/atom range). Dispersion of these projections is not significant and the reason of this is the small scattering angles of atoms channeled through the CNTs.

References

1. D.W. Brenner, O.A. Shenderova, J.A. Harrison, S.J. Stuart, B. Ni, S.B. Sinnot. "A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons", J.Phys: Condens. Matter, 14, pp.783-802 (2002)

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