SIMULATION OF CHANNELING IN CARBON NANOTUBES

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One of the most important methods for the study of nanomaterials is the construction of computer models (see, eg [1]).In this paper we study some questions channeling of atomic and molecular structures of carbon nanotubes. Depending on the task used a wide range of models. For analytical estimates apply the model nanotubes with a continuous potential. Models of nanotubes with the fixed position of the atoms of the tube except for a single atom, the nearest to the moving particles with high speed and allow us to calculate parameters such channeling, a critical angle of channeling, the spread in angles and coordinates of the flight. Models that take into account the dynamics of all atoms of the nanotube, are suitable for occupancy studies of nanotubes atomic and molecular structures for the evaluation of the energy loss in the interaction with atoms of the nanotube, as well as to explore issues of defect. Among these models we consider a model nanotube when each atom is fixed in a parabolic potential well, as well as a model in which bonds between atoms are "spring" and a model with many types of Tersoff-Brenner potentials. The result of modeling was a reaffirmation of an earlier opportunity (Osipyan Y.A) filling CNTs with hydrogen to a much greater extent than is achievable with standard physical and chemical methods. Some results of these studies were partially reported at the conferences held in 2009 (see, eg [2]).

References.

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