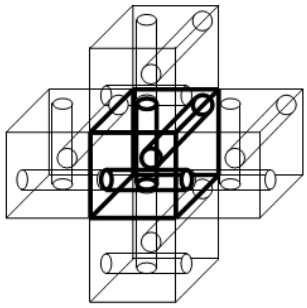
Hydrogen sorption process modeling on the periodic structures formed by carbon nanotubes

Slepicheva M.[1], Chernyshev Y.[1], Basteev A.[1], Bazyma L.*[1], Ugryumov M.[1]

[1]*National Aerospace University, 61070, Kharkov, Ukraine*
**e-mail: bazima@htsc.kipt.kharkov.ua*

The process of molecular hydrogen physical sorption on the surfaces of carbon nanotubes (CNT) which are forming the spatial pattern is interesting from mathematical point of view and numerical simulation of above process has scientific interest as well [1]. The cell of computational region (see Fig.) in which three or mutually orthogonal CNT without intersection are replaced was considering for simplification.



Cells periodic structure.

The molecular hydrogen as the model particles are sited in the cells. All involved in consideration model particles have rectangle-shape potential that gives us the opportunity to use the event-driven simulation method [2]. The hypothesis about periodical conditions on the region borders was assumed and it physically means that infinitely long CNT are closely interwoven one with another [3]. The model particles are supplied from selected facet of cells system. The percentage of sorbet hydrogen molecules at high temperatures was calculated taking into account single sorption layer only. The reducing of system temperature after initial filling and with primary adsorption layers formation has been proposed with the aim to suppress the re-adsorption process.

The results of numerical investigations of defects-vacancies influence in the CNT structure on the sorption capability at different thermo dynamical conditions were obtained on the base of proposed method.

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[3] M. Slepicheva, Proceedings of the International Scientific Conference of Students and Young Scientists, Kyiv: Bukrek, 294 (2011).