Molecular Simulation of Hydrogen Storage in SWNT

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Since the suggestion of high efficiency storage of hydrogen with single walled nanotubes (SWNTs) by Dillon et al. [1], experimental determinations of the storage capacity and mechanism of storage have been extensively studied. Hydrogen storage capacity of high purity SWNT was reported to be more than 8 wt % at 120 bar and 80 K [2], and 4.2 wt % at 100 bar at room temperature [3].

In this report, the effective adsorption mechanism of SWNT was studied through molecular dynamics simulations. A bundle of (10,10) SWNT was modeled as shown in Fig. 1. Assuming the simple adsorption of hydrogen to the surface of SWNTs, potential forms between H2-H2 and C-H2 were both expressed by Lennard-Jones functions. Fixing the relative coordinates of carbon atoms to the center of mass of each SWNT, the center of mass motion was modeled with the van der Waals force between them. As shown in a snapshot in Fig. 2, the preliminary calculation showed the absorption of hydrogen molecules in-between each SWNT as suggested by ref. [2]. The simulation of this phase change process was not possible within possible calculation time for reasonable van der Waals force between each SWNT. A suitable acceleration of the simulation of phase change process will be discussed.

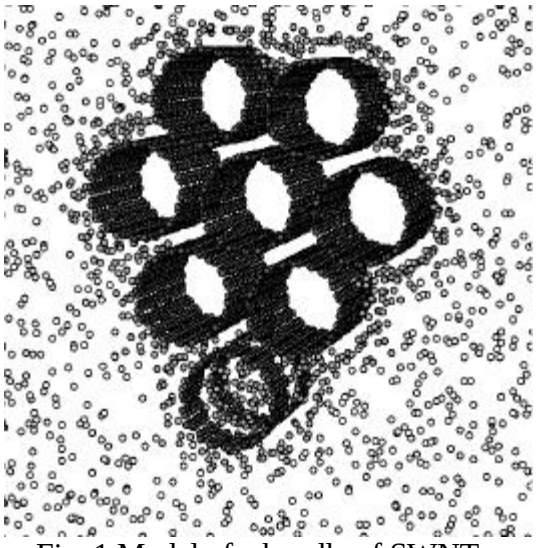

Fig. 1 Model of a bundle of SWNTs.

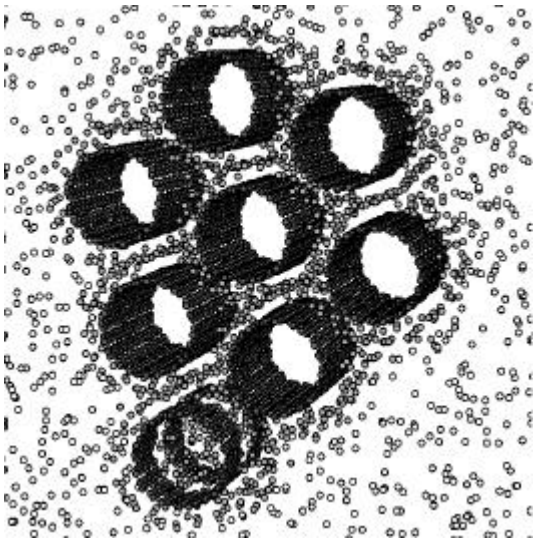

Fig. 2 Adsorption of hydrogen molecules in-between each SWNT.

References:

[1] A. C. Dillon et al., Nature, 386 (1997), 377.
[2] Y. Ye et al., Appl. Phys. Lett., 74-16 (1999), 2307.
[3] C. Liu et al., Science, 286 (1999), 1127.