A Molecular Dynamics Simulation of Hydrogen Storage by SWNTs

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The mechanism of efficient hydrogen storage [1] with SWNTs [2,3] was studied through classical molecular dynamics simulations. Assuming the physical adsorption of hydrogen to the surface of SWNTs, potential forms between H_2-H_2 and C-H_2 were both expressed by Lennard-Jones functions. Each SWNT was regarded as rigid molecule and van der Waals potential between SWNTs was derived as Lennard-Jones (8-4) function by integrating potential between carbon atoms. As shown in Fig.1, 7 SWNTs were placed in a fully periodic system, so that a SWNT exactly continues in the longitudinal direction.

During 500 pHs simulation for 77K and 15 MPa, the adsorption was observed only outside of bundles as shown in Fig. 2(a). In order to realize the adsorption between SWNTs within reasonable simulation period, the van der Waals potential between tubes was once decreased to 1/50, then hydrogen molecules rapidly intruded between SWNTs by expanding the bundle of SWNTs as shown in Figs. 2(b) and 2(c). By restoring the van der Waals force, the adsorption structure remained almost unchanged. Similar simulations were performed for (8,8) and (12,12). The number of finally adsorbed hydrogen molecules was almost proportional to the number of carbon atoms, and the storage amount became about 5 wt % regardless of the tube radius.

In order to estimate the adsorption to the tube interior, a bit shorter SWNTs was simulated. Fig. 3 shows the final absorbed structure. The number of absorbed hydrogen molecules was almost proportional to the volume of interior space. While the amount in weight percent of hydrogen adsorption inside SWNTs increased with increasing diameter, adsorption between tubes was almost constant. Total amount of hydrogen adsorption for 77K and 15 MPa system was predicted as 6.9, 7.7, and 8.1 wt % for (8,8), (10,10), and (12,12) bundles, respectively. These predictions were almost consistent with the experimental adsorption amount by Ye et al. [4].

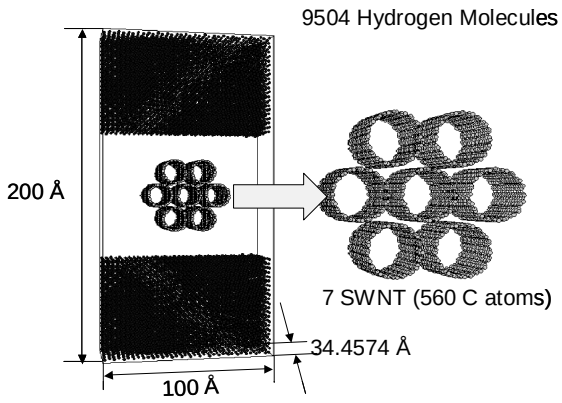
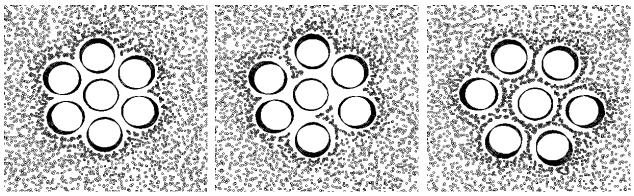
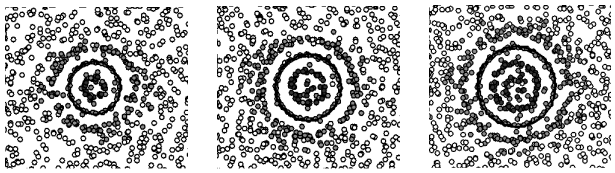


Fig. 1 Initial configuration of a bundle of (10,10) SWNTs.



(a) 500 ps (b) 510 ps (c) 1000 ps

Fig. 2 Hydrogen strage between SWNTs.



(a) (8,8) (b) (10,10) (c) (12,12)

Fig. 3 Hydrogen storage inside each SWNT.

References:

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