Rapid Water Transportation through One-dimensional Carbon Nanospaces

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~~ABSTRACT :~~ Water transportation through one-dimensional (1D) and quasi-1D internal nanospaces ~~were directly observed by the rates of water vapor adsorption in the internal nanospaces~~ of highly pure single- and double-~~-~~wall carbon nanotubes, respectively, was directly investigated from the rates of water vapor adsorption in the~~that have quasi-1D and 1D~~ nanospaces~~, respectively~~. Water was found to be~~is rapidly~~ transported more rapidly through 1D nanospaces ~~rather~~ than through quasi-1D nanospaces. Molecular dynamics simulations of water transport through carbon nanotubes were found to agree with~~shows the same tendency as~~ the experimentally determined adsorption rates. In a 1D system, fewer hydrogen bonds are formed between water molecules ~~rarely form hydrogen bonding between water molecules~~. This results in~~Therefore, the~~ rapid water transport~~ation~~ through~~is a result of less hydrogen bonding formation of water adsorbed in~~ 1D nanospaces.

Water is one of the most ubiquitous substances, and it is well known to have anomalous physical properties owing~~due~~ to its constituent hydrogen bonds~~ing~~. Hence, the anomalous properties of water have been ~~continuously~~ studied extensively.~~-~~[1] Water transportation through a water channel in a biomembrane is another important research topic~~issue~~, because a water channel is involved in many physiological processes. Water channels have narrow hydrophobic nanospaces.~~-~~[2] Because~~As~~ these channels have~~are~~ flexible and complex structures, a nanoporous material having a model ~~structure for a~~ water channel structure is required in order to understand water transport~~mechanism~~ through~~via~~ a water channel. A ~~C~~carbon nanotube (CNT) is believed to be an ideal~~ly~~ model ~~structure of a~~ water channel structure because it has~~due to having~~ hydrophobic one-dimensional (1D) nanospaces.[3] Thus, in recent times, the properties of water ~~properties~~ in CNTs~~carbon nanotubes~~ have been~~are actively~~ studied actively~~recently~~.~~-~~[4] ~~The w~~Water permeation through membranes fabricated using~~by~~ CNTs~~carbon nanotube~~ is demonstrated to study the working of a water channel~~ mechanism~~.[4] However~~Nevertheless~~, the mechanism of water transportation through the internal nanospaces of carbon nanotubes remains~~is still not~~ unclear.

Ideal single- and double-~~-~~wall carbon nanotubes (SWCNTs and DWCNTs) were synthesized by Hata et al. and Endo et al., respectively; these CNTs were found to~~those~~ have extremely low metal catalysts, long aspect ratios, and hydrophobic internal nanospaces.~~-~~[5] These carbon nanotubes are ideal for~~have the great advantage of~~ fundamental studies~~y~~ on water transportation through ~~the~~ internal nanospaces. Here, we use these SWCNTs and DWCNTs to demonstrate~~directly show~~ water vapor transportation through their nanospaces based on~~these carbon nanotubes by~~ the rate of water vapor adsorption ~~in SWCNT and DWCNT,~~ and molecular dynamics (MD) simulations.

The SWCNTs and DWCNTs were observed by ~~H~~high-resolution transmission electron microscopy (HRTEM) ~~observations were performed on SWCNT and DWCNT~~ using JEM-2100F (JEOL Co.) at 120 kV. The ~~A~~adsorption rates of water vapor were measured at 303 K every 50 ms using a ~~home~~custom-made volumetric apparatus. ~~Here, t~~These CNTs~~carbon nanotubes~~ were~~are~~ heated at a pressure less than~~<~~ 0.1 Pa for 2 h prior to the adsorption rate measurements. MD simulations with the leapfrog time integration scheme were performed to~~for~~ understand~~ing~~ the water transportation through the carbon nanotubes; the model comprised a single SWCNT having infinite length and a diameter~~s~~ of 1 or 2 nm, placed in a unit cell having dimensions of 4 × 4 × 6 nm^3. The interaction potentials between water molecules and between a water molecule and a carbon wall were calculated ~~by~~ using TIP5P and Lennard-Jones potential models, respectively. ~~Here, t~~The TIP5P potential model, proposed by Mahoney et al., ~~is~~ combines~~ation model of the~~ dispersion and electrostatic interactions~~, and it was proposed by Mahoney et al~~.~~-~~[6] A complete MD simulation (100 ps) was conducted at around~~close to~~ 303 K for~~using~~ an integration time of 0.1 fs (~~The~~ simulation procedures are presented in detail in Supporting Information~~.~~).

Figure 1 shows ~~the~~ HRTEM images of the DWCNTs and SWCNTs. The average internal diameter~~s~~ of the DWCNTs and SWCNTs is~~are~~ 1 and 2–3 nm, respectively, as reported previously~~which are also shown in the preceding papers~~.~~-~~[7] Water vapor~~s~~ can be adsorbed mainly in the internal nanospaces, because~~as~~ these CNTs~~carbon nanotubes~~ form bundles. Thus, SWCNTs and DWCNTs act as~~produce~~ typical 1D and quasi-1D systems, respectively, for water~~, respectively~~. Figure 2(a) shows changes in the fractional filling ~~changes~~ of water with time ~~progress~~. Water vapor~~s~~ is~~are not~~ adsorbed from~~below~~ 0.1 s onward,~~ then begin to be adsorbed at that time,~~ and finally, ~~achieve~~ equilibrium fractional filling~~s~~ is achieved. The fractional filling~~s~~ of water vapor for the 1D system ~~were significantly~~ increased rapidly from 0.5 to 10 s, whereas that~~while these~~ for the quasi-1D system ~~were gradual~~ increased gradually. Therefore, water molecules are transported more rapidly ~~transport~~ through 1D nanospaces ~~rather~~ than through quasi-1D nanospaces. The ~~A~~adsorption rates of water vapor were evaluated from the differential change in the fractional filling~~ change~~, as shown in Figure 2(b), which is directly indicative of~~show the~~ water vapor transportation~~s~~ through 1D or quasi-1D nanospaces. We observed ~~E~~extremely fast adsorption of water vapor below 0.2 s,

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relatively fast adsorption from 0.2 to 10 s, and gradual ~~progress of~~ adsorption above 10 s~~ were observed~~. Fast adsorption below 0.2 s is caused by diffusion~~a result~~ of water ~~diffusion ~~into the internal nanospaces. ~~The r~~Relatively fast and gradual adsorption is caused by~~process should result from~~ water vapor transportation through the nanospaces. From 0.2 to 10 s, water vapor is adsorbed faster in 1D nanospaces than ~~I~~in ~~comparison with ~~quasi-1D nanospaces~~system, faster adsorption in 1D nanospaces is actually observed from 0.2 to 10 s~~.

The results of MD simulations of water in the internal nanospaces, shown in Figure 3, clarify~~demonstrates~~ the mechanism of water vapor transportation through the 1D and quasi-1D nanospaces~~, as shown in Fig.3~~. The ~~absolutely different~~ time scale used in~~between~~ the experiment and in the MD simulation is completely different because of the~~due to~~ different CNT lengths~~ of carbon nanotubes~~. Figure 3 also shows photographs~~the snapshots~~ of water transportation~~s~~ through the 1D and quasi-1D nanospaces. Water molecules are located on~~situated in~~ the left-hand side in the~~of~~ carbon nanotubes at 0 ps, following which they~~and then~~ begin to flow toward the right-hand side. The ~~F~~fractional filling of water is calculated from the number of water molecules~~ar number~~ o~~i~~n the right-hand side. Water ~~rapidly ~~transport~~s~~ toward the right-hand side is much faster in a~~the~~ CNT with a diameter~~carbon nanotube~~ of 1 nm than in a~~diameter, while water transportation for~~ quasi-1D nanospace~~ is considerably slow~~. In a CNT with a diameter of~~Thermal diffusivity for~~ 1 nm, the thermal diffusivity~~diameter quickly~~ increased rapidly with oscillation~~. On the other hands~~, whereas in a CNT with a diameter of~~the increase of thermal diffusivity for~~ 2 nm, it increased~~diameter is~~ moderately. After 10 ps, ~~T~~the thermal diffusivity~~ies~~ of water vapor is~~are~~ 28×10^{-9} $\mathrm{m^2\ s^{-1}}$ for a 1D nanospace and 4×10^{-9} $\mathrm{m^2\ s^{-1}}$ for a quasi-1D nanospace~~ in 10 ps~~. However, after 70 ps, the respective thermal diffusivities ~~for 1D and quasi-1D nanospaces ~~are 40×10^{-9} and 28×10^{-9} $\mathrm{m^2\ s^{-1}}$~~ in 70 ps, respectively.~~ (see Supporting Information). These values agree~~tendencies correspond~~ with the experimental adsorption rates~~, as~~ shown in Figure 2. The ~~N~~numbers of hydrogen bonds~~ing~~ is~~are~~ evaluated from the photographs~~snapshots~~, as shown in Figure 4. In the 1D system, the number of hydrogen bonds~~ing~~ remains~~is~~ constant ~~at ~~(0.4) during the calculation time step. In the quasi-1D system, the number of hydrogen bonds~~ing is~~ increases~~d~~ from 1 to more than~~and over~~ 3 in 50 ps. In other words~~That is~~, water molecules cannot form an adequate number of hydrogen bonds~~ing~~ in the 1D system. ~~Hence, h~~Hydrogen bond~~ing~~ formation hinders~~prevents from~~ water transportation through 1D nanospaces, which otherwise~~because 1D nanospaces~~ provide a path for rapid water transportation, as mentioned above.

In this study~~paper~~, we investigated direct water transportation through 1D and quasi-1D nanospaces~~ were observed~~. Water vapor was found to~~rapidly~~ transport~~s~~ more rapidly through 1D nanospaces ~~rather ~~than through quasi-1D nanospaces, which is in agreement with the~~supported by~~ MD simulation~~s~~ results. Hydrogen bond~~ing~~ formation in~~of~~ water molecules is restricted in the~~by~~ 1D nanospace. Therefore, ~~as a result of restriction of hydrogen bonding formation ~~water molecules rapidly transport through the 1D nanospaces.

~~ASSOCIATED CONTENT~~

SUPPORTING INFORMATION. N2 adsorption isotherms at 77 K for SWCNTs and DWCNTs, and analysis of~~the~~ nanospace structure~~ analysis~~. Water vapor adsorption isotherms at 303 K and thermal diffusivities of water by MD simulation. This material is available free of charge via the Internet at

http://pubs.acs.org.

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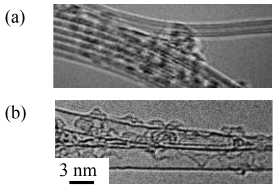

Figure 1. TEM images of DWCNT (a) and SWCNT (b).

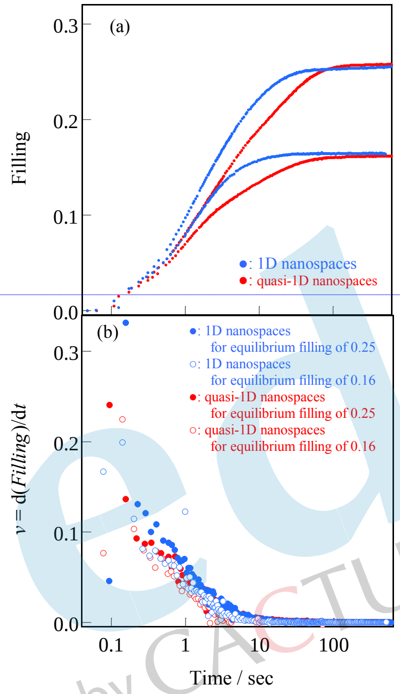

Figure 2. Changes in fractional ~~F~~filling ~~changes~~ and rates of water vapor adsorption~~bed~~ in the internal

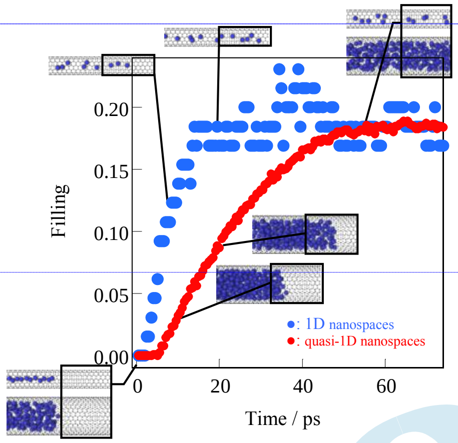

Figure 3. Simulated changes in fractional filling ~~changes~~ of water molecules in internal nanospaces of CNTs~~carbon nanotubes~~. Water molecules flow from the left to the right side in the CNTs~~of carbon nanotubes to the right side~~.

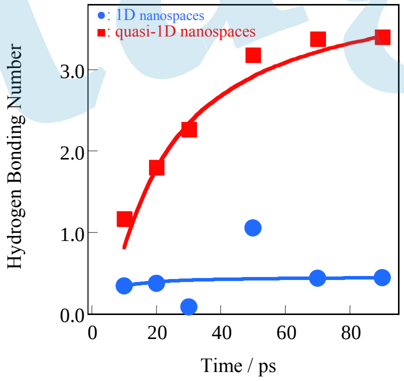

Figure 4. Changes in the ~~N~~number ~~changes~~ of hydrogen bond~~sing~~ with time~~ progress~~.

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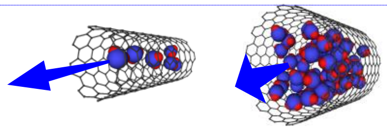

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