

Storing of noble gases on Carbon Nanotubes with the method of molecular dynamics

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ABSTRACT

Carbon Nanotube was discovered by Japanese Somioljima in 1991. After two years of few wall nonotubes, one wall nanotube was discovered. Carbon nanotube is of great importance because of its structural characters. Its different applications are of great consideration.

Storing of noble gases i.e. Xenon, Krypton and Argon are of great consideration. Because of high space and porosity, Carbon structures are known as the ideal matter for the absorption of gasses in nano scale.

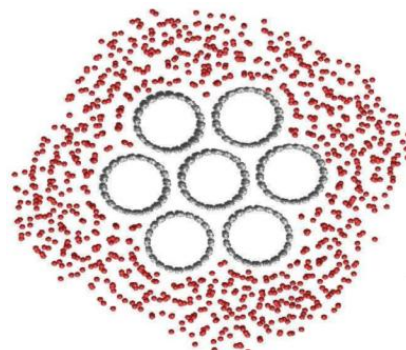
Carbon nanotubes are of great internal volume and space for absorption and storing of gasses than Carbon nano cones of same number of carbons.

In this article storing of noble gasses on carbon nanotubes with the method of molecular dynamics is experimentally investigated. In isolated case, absorption of Argon, Krypton and Xenon gases on nanotube in different temperature and different Pressure is calculated.

1. General

Absorption of noble gases (Xenon, Krypton and Argon) on carbon nanotubes with the method of the dynamics of molecules has been investigated in NVT. Similar compounds for Xenon, Krypton and Argon gases have been investigated in different temperatures and their absorption amount has been measured in saturated case, using Tinker software. Physical quantities namely place and velocity have been determined (numerical calculations) by Beeman algorithm [3.2]. The temperature of the system is arranged getting benefit of Nose-Hoover thermostat and interactions are placed by MM₃ field force.

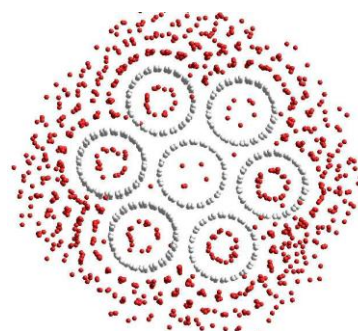
The performed studies and investigations explain that carbon nanotubes are made in general from nanotubes whose diameters are closed to (10.10)nanotube diameter. Because of this, in this article we wanted to come close to an actual model so we had the sum of (10.10) nanotube in which seven nanotubes with ten unit cells laying on the axis of nanotube which has 2800 carbon atoms. In the first configuration of similar compound 100 to 2300 atoms of noble gas atoms distributed accidentally on the external part of the nanotubes and similar compounds took place in different temperatures (1 figure). Periodic boundary conditions are used in every three dimensions and their radius is taken in to account 12.5 Angostroms . Getting benefits of dynamic method of the system in NVT the absorption amount is measured. To reach absorption amount of the system to equilibrium similar compound is continuing till its amount is constant. Duration of one similar compound is famto second. This quantity is less than hundred pico second and is in saturated case and than first configuration has reached to equilibrium in hundred picosecond [4].



(figure 1) accidentally distribution on the external part of the sum of nanotubes (first configuration of similar compound) is shown.

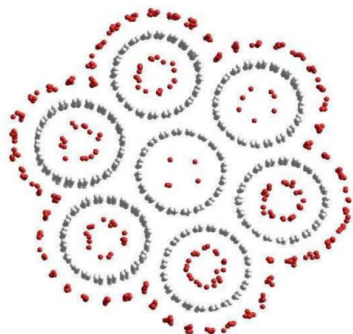
2. Results of similar compound

Results of similar compound show that gas atoms at first accumulated on external walls of nanotubes as a layer at low pressure. With the enhancement of gas pressure, gas atoms are accumulated as many layers on external walls and slowly, the enter space of nanotubes became full up to it reaches the saturated case. In (figure 2), it is observed that the atoms of gas can be absorbed on internal and external part of nanotubes [4].



(figure 2). Absorption of gas atoms on internal and external part of the sum of nanotubes (final configuration of similar compound) is shown.

For the determination of the amount of absorption we only take in to account the first absorbed layer and calculate the atoms related to it (figure 3). Looking in to account the amount of absorption, number of absorbed atoms has been explained at carbon atoms.

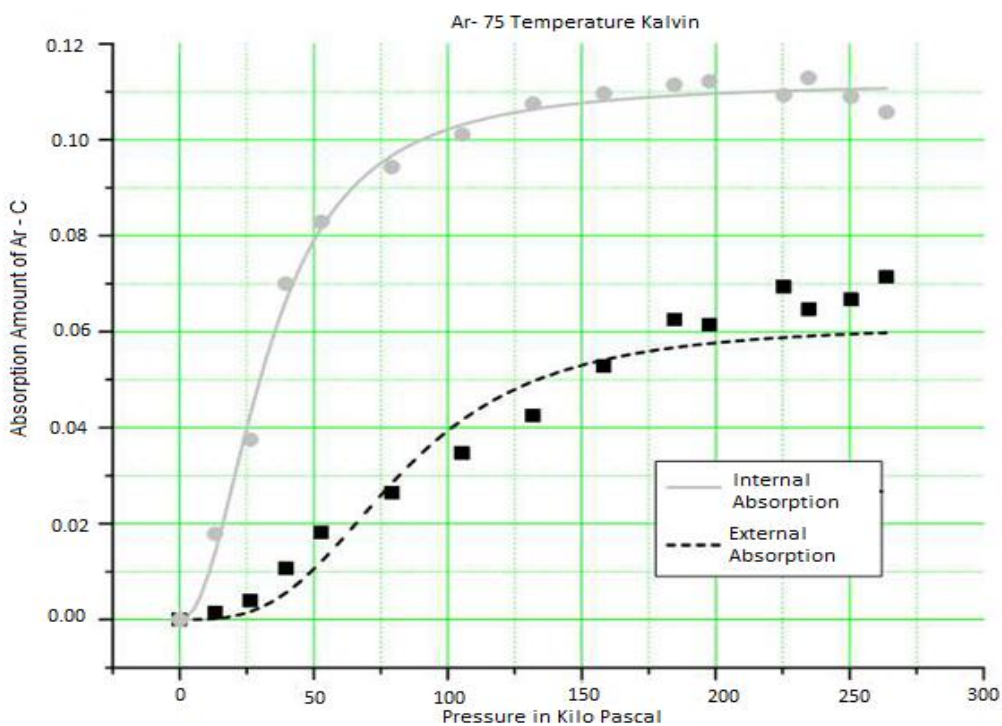


(figure 3). Atoms of gas have been absorbed on internal space and external part of the sum of nanotubes.

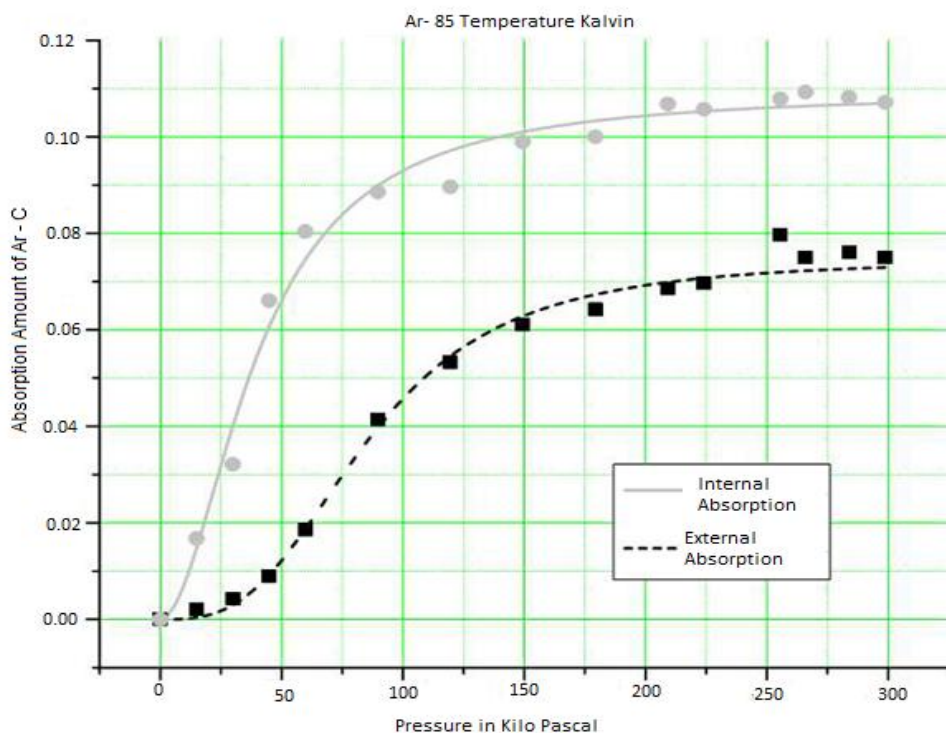
Absorption of similar compounds on the sum of nanotubes are investigated for Xenon gas is in 110, 120 and 130 Kelvin temperatures, absorption amount of Krypton is in 75, 85 and 95 Kelvin temperatures and for Argon is in 75, 85 and 95 Kelvin temperatures.

The obtained results are: with the enhancement of pressure, amount of absorption is enhanced. The enhancement of absorption because of the enhancement of pressure is also absorbed in the previous theory[5,1]. With the enhancement of temperature, absorption amount of the gas inside the nanotubes is enhanced. On the other side, with the enhancement of temperature, a small amount of gas is absorbed on the external wall of nanotubes. It is clear that the kinetic energy of gas atom is enhanced with the enhancement of temperature. In (figure 4 a, b, c), amount of absorption of Argon gas at different temperatures is shown on the external and internal part of nanotubes. Here we take in to account the figure of Argon only and the amount of absorption of gases is in Table 1.

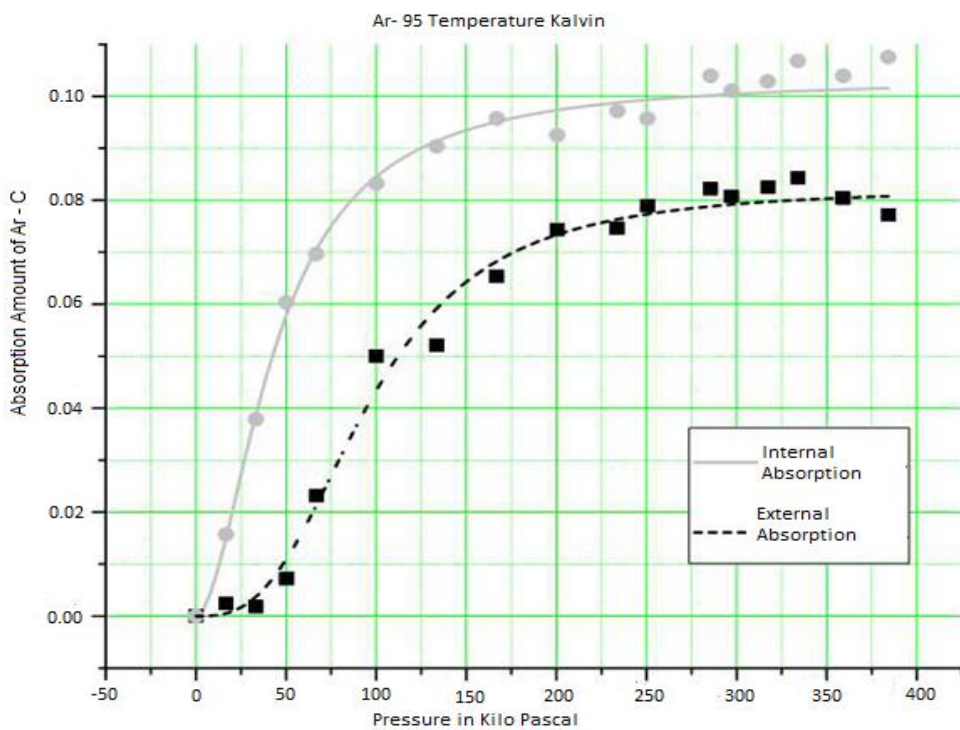
Our investigation shows that the carbon junctions are enhanced hundred times with enhancement of heat.



(a)



(b)



(c)

(figure 4 a,b,c). Comparison of Argon gas in different temperatures on the external and internal part of nanotubes has been shown.

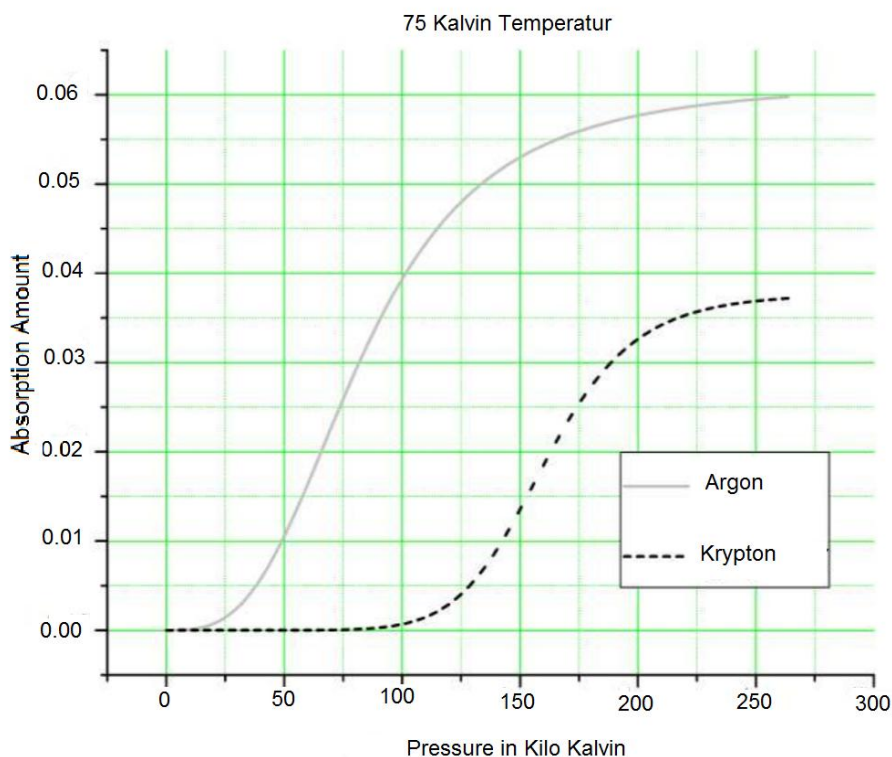
(Table 1).Absorption amount in saturated case at different temperature.

	Temperature (Kalvin)	External Absorption	Internal Absorption
Xenon	110	0.044 Xe-C	0.089Xe-C
	120	0.046 Xe-C	0.088 Xe-C
	130	0.050 Xe-C	0.086 Xe-C
	75	0.038 Kr-C	0.097 Kr-C

Krypton	85	0.050 Kr-C	0.095 Kr-C
	95	0.055 Kr-C	0.092 Kr-C
Argon	75	0.060 Ar-C	0.110 Ar-C
	85	0.073 Ar-C	0.107 Ar-C
	95	0.080 Ar-C	0.102 Ar-C

It is obtained from the investigations that the atomic radius of gas has effect on the amount of absorption. Atomic radius of Argon is smaller than the atomic radius of Krypton and that of Krypton is smaller than the Xenon, the smallest the radius the

greatest is the absorption, so we can say that Argon is more absorbed than Krypton and Xenon. The amount of absorption of Argon and Krypton gas At 75 Kelvin temperature inside nanotubes is shown in (figure 5).



(figure 5). The amount of absorption of Argon and Krypton gas At 75 Kelvin temperature is estimated inside nanotubes.

3. Conclusion

Results of similar compounds indicate that there is great absorption of noble gases on the collection of open nanotubes and carbon nanotubes have the capacity of absorbing gas atoms on the internal space and outer area of nanotubes. In

saturated case, with the enhancement of temperature, gas absorption decreases on external wall of nanotubes and increases on its internal space. With the reduction of atomic radius, the absorption amount increases.

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