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Surface adsorption of carbon monoxide and hydrogen gases mixed with boron nitride (7 ,7) nanotubes by Monte Carlo method

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Abstract

In this project, the pure adsorption of mixtures of hydrogen and carbon monoxide on nanotubes (7 and 7) of boronitrile nanotubes was studied by Montecarlo method. The potential for the interactions of gases with each other and with a nanotube according to the Lennard-Jones equation and its parameters are calculated according to Lawrence-Bartwell rules for interaction between gas, gas and gas-nanotubes. Simulation of adsorption of gases at different temperatures and pressures and the results of gas adsorption density are calculated and compared in each case. The results show that the adsorption of gases is directly related to the increase of pressure and with the increase of temperature, the relation is opposite. Comparison of the results shows that absorption is higher in pure state.

Keywords: Surface adsorption, single-wall nano-tubes of boron nitride, Monte Carlo simulation, density, carbon monoxide gas and hydrogen

1. Introduction

Today's world is the era of substructures and our goal is to achieve self-sufficiency and independence in this area. Technology, technology, and nanotechnology. The first nano spark during a Fayman lecture, with the statement that "there is a lot of space at a low level" was introduced for nanotechnology. He It has been suggested that individual atoms can be manipulated and produce small materials and structures that have different properties [1]. So, after nearly a year, today, it has achieved

the capabilities of this human technology that has brought about economic life, life improvement and the development of science. Monte Carlo molding In the center of the set, where N has a constant particle, the energy comes from the interaction of particles from the substrate [2]

$$U = \frac{1}{2}\int_{i=1}^{N}\int_{j\neq i=1}^{N} Uij$$

(Equation 1) is used for the absorption or separation of various types of gases on a variety of nanotubes using Monte Carlo method from the Lennard-Jones potential [3]. The equation for the interaction of gas with the wall of the nanotube is as follows

$$U_{gn} = \varepsilon_{gn}\sum_{i=1}^{N_{gas}}\sum_{j=1}^{N_{nanotube}}\left[\left(\frac{б_{gn}}{r_{ij}}\right)^{12} - \left(\frac{б_{gn}}{r_{ij}}\right)^{6}\right]$$

(Equation2)

Ngas The number of gas molecules in the N nanotube box, = the number of nanoparticle molecules

〖E_ (gn,) 〖b〗 _ (gn)〗 _ = The energy and longitudinal parameters of the Lennard-Jones potential in the interaction of gas molecules with the nanotubes and rij = the particle distance between particles i and j.And the potential equation for gas-gas interactions is as follows:

Equation3

$$U_{ij} = 4\varepsilon_{gg}\left[\left(\frac{б_{gg}}{r_{ij}}\right)^{12} - \left(\frac{б_{gg}}{r_{ij}}\right)^{6}\right]$$

ggε and ggb are the energy and volatility parameters of the Lennard-Jones potential for interactions of gas-gas molecules, respectively. The value of the potential parameters for the interaction of gases with boron nitride nanotubes is obtained from the article in question [4] using the Lorenz-Bertwell law (Equation 4)

$.б_{ij} = \frac{б_i + б_j}{2}$ $\varepsilon_{ij=}\sqrt{\varepsilon_i\varepsilon_j}$ (Equation 4)

Using the Metropolis technique, generators of random numbers [1 and 0] are produced in the computer software environment. The nanotube cartoon coordinates can be obtained from the Internet, the tubegen site or the Nanotube modeler software, and by using the Gaussview software, the nanotube was designed and simulated at the center of the cell. Therefore, the initial arrangement of the simulation is done.

2. Computational data

The dimensions of the box are considered according to the tube length and diameter of 100 × 100 ×

100 Angstroms, and the number of molecules in the box in accordance with the ideal gas equation is obtained and placed in the program.

The average density is calculated in this program, so the length of the tube does not have much effect on gas absorption. In general, the following conditions are considered in the calculations performed.

The length of the nanotube is 60 angstroms and the number of boron and nitrogen atoms is 700

- The nanotube is positioned in the middle of the simulated box to maintain symmetry and not affect the direction of the matter.
- Nanotubes are rigid and gas molecules in the form of butter, to be considered for the interaction of pure gases with nanotubes [5, 6]
- Vibration of boron and nitrogen atoms is neglected so that geometric change does not affect the simulation process.
- Boundary boundary conditions have been applied to the determination of the effect of simulation tubes on calculations [7]
- The Monte Carlo simulation technique is used with the metropolis algorithm in the N, V, T system for initial configurations.
- The system returns to equilibrium after 107 cycles.

3. Calculations and results

The distribution of hydrogen gas in a mixture of two gases with different molar percentages at 350 ° C and 8 MPa pressure is investigated. According to the calculations, concentration has a direct correlation with the absorption rate. The point to be noted is that at a concentration of 100% hydrogen gas, the adsorption density is greater than 4 at 25% concentration. The reason is to look for gas mixing because the gases are in the mixed state, they interact with each other and absorb the nanotubes. Figure 1 also confirms this impression.

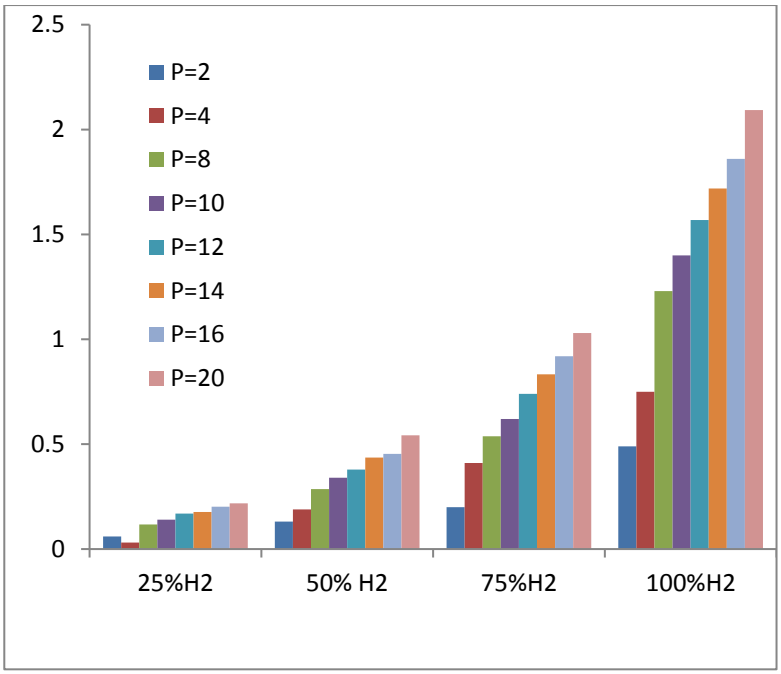

Figure 1) Comparison of absorption in different molar percentages at 250 ° K)

In Figures 2 and 3 of the calculations, the comparison of the adsorption of gases in the pure state and the mixture at constant temperature with the same number of gases is carried out in the pure state of absorption, and this difference is well observed in the first layer of adsorption. It can be concluded that the interaction of gases together prevents the gas from absorbing with the nanotubes.

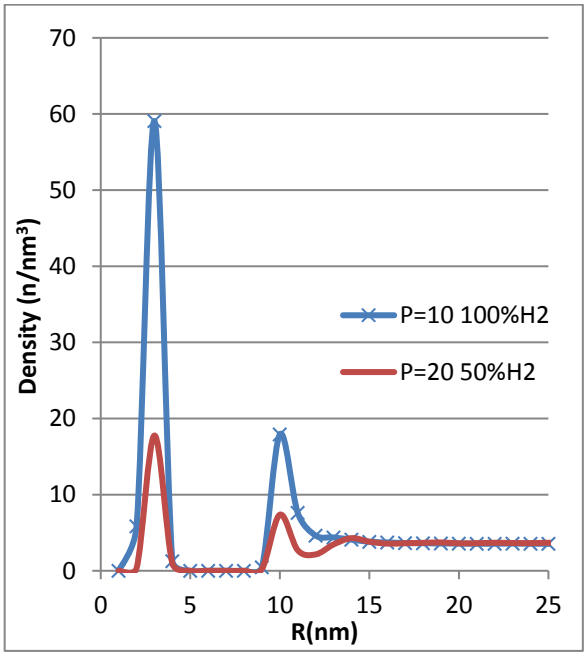

Fig. 2) Comparison of pure hydrogen adsorption density and mix at constant temperature)

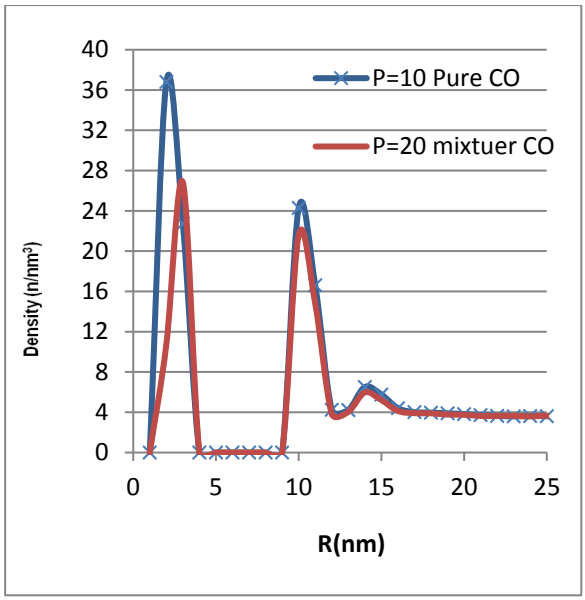

Fig. 3) Comparison of pure carbon monoxide adsorption density and mix at constant temperature)

In the past, carbon monoxide and hydrogen gas absorption has been investigated in a dual mixture of carbon nanotubes by the GCMC method. The results have shown that carbon monoxide adsorption is always higher [8].

.In this study, we investigated the absorption of these two gases on boron nitride nanotubes

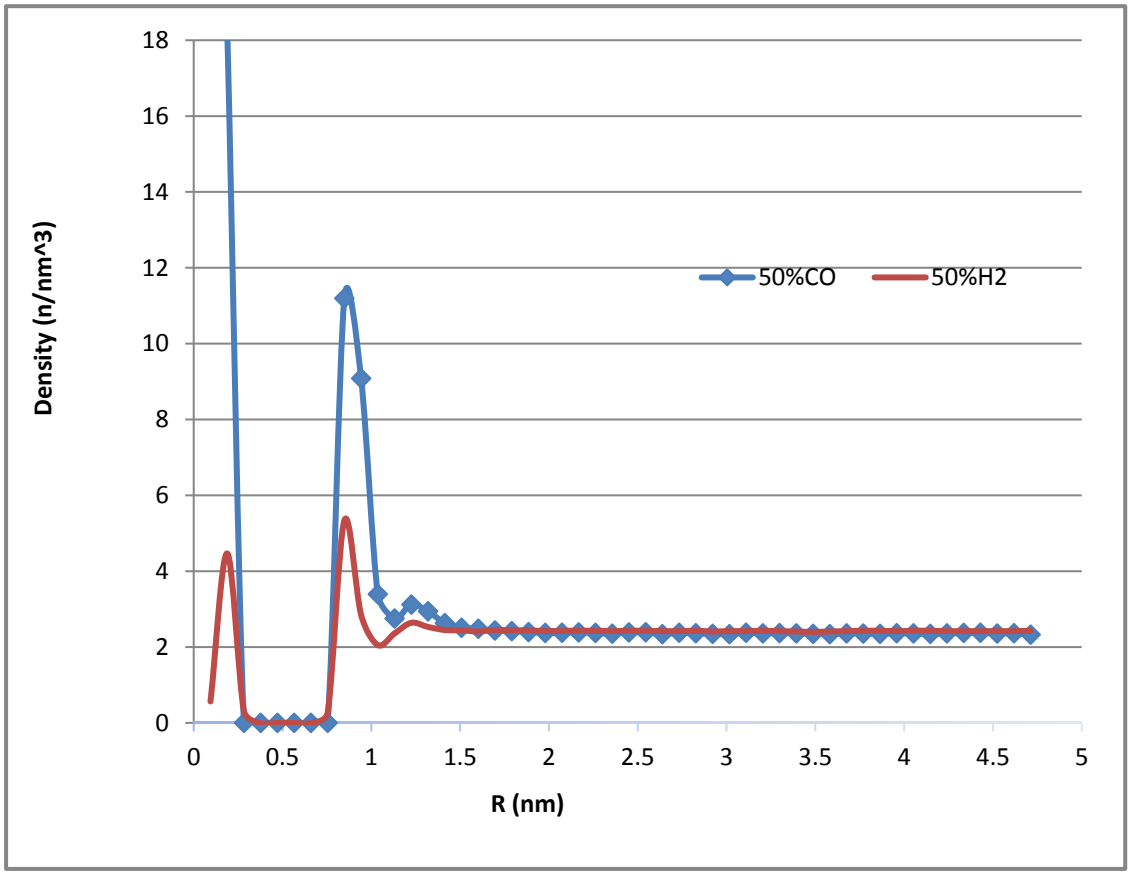

Fig. 4) Comparison of Surface Absorption Between Gashydrogen and Carbon Monoxide)

According to the calculations carried out at 300 K ° and 20 Mpa, the absorption of two gases (under the same conditions) is obtained according to Fig. 4. The results show that carbon monoxide gas

adsorption is clearly higher than hydrogen. The reason for this is the more intense interaction with the nanoparticle, since the potential parameters and the size of the carbon monoxide molecule are higher than that of hydrogen. Chart 5 compares the weight percentages of both gases. Researchers such as Ma and his colleagues reported the percentage of stored hydrogen stored at room temperature and pressures of 10-0 Mpa in multi-layer boron nitride 2.6% [9]. And Tang and colleagues reached a 4.2% result in multi-layer nanotubes [10]. In the article, the percentage of hydrogen storage in bomber boronatriates was reported by 2.6% [11]. In this study, we found more than 2.66% in the single-wall boron nitride nanotubes. In this project, the percentage of carbon monoxide gas storage in a single boron nitride nanotube was at 200 kPa and 20-20% MP 20 pressure.

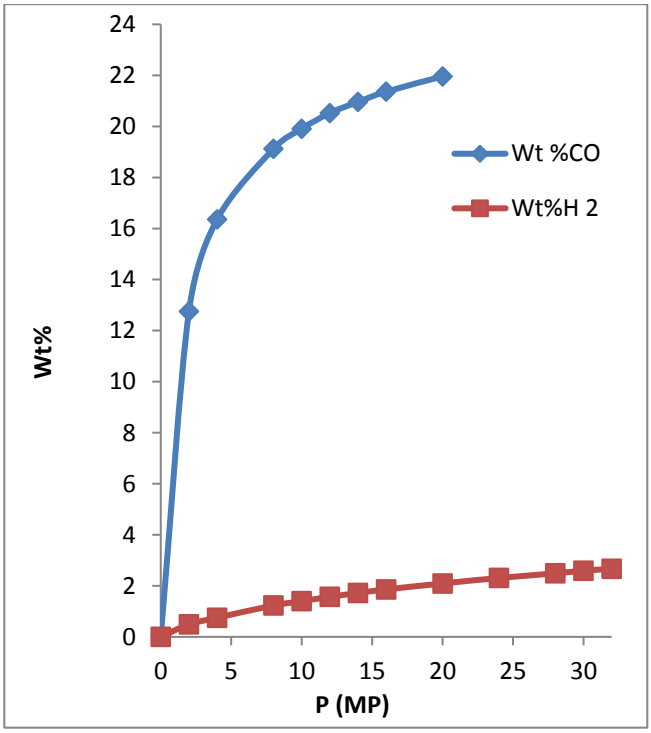

Chart 5) Comparison of the weight percent of hydrogen and carbon monoxide at 200 K and various pressures)

By calculating the relative percentages of hydrogen uptake, the numerical value is 5.726% at 200 ° K and compared with the relative percentage of carbon monoxide, ie 6.65%. Consequently, carbon monoxide is more absorbed, and these two gases can be separated.

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