Microelectronics Journal 41 (2010) 142–149

Contents lists available at ScienceDirect

Microelectronics Journal

journal homepage: www.elsevier.com/locate/mejo

Alcohol sensors based on SWNT as chemical sensors: Monte Carlo and Langevin dynamics simulation

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ARTICLE INFO

Article history:
Received 26 August 2008
Received in revised form
25 January 2010
Accepted 25 January 2010
Available online 21 February 2010

Keyword:
SWNT
CH_3OH and C_2H_5OH
Monte Carlo (MC) simulation
Langevin dynamics (LD) simulation

ABSTRACT

In this research the decomposition products of the alcohol gases and their decomposition stages at the surface of the elements of single walled carbon nanotube (SWNT)-based powder are analyzed. The SWNT-based powders catalytically oxidized ethanol and methanol. The nano-crystalline and nanotubes have low band gaps and high mobility, thus offer applied potential as gas adsorption. Interaction between alcohol molecules and SWNT is investigated using Monte Carlo (MC) and Langevin dynamics (LD) simulation methods. We study the structural, total energy, thermodynamic properties and the acceptance ratio of methanol gas passing through an: armchair SWNT (4, 4) at different temperatures. Passing gas in SWNT changed the properties of it, in this research we have calculated the electrical and structural charges, in addition, transfer of charges from atoms to SWNT was investigated and it was found that there is a direct relation between the total energy and temperature.

We study the structure, total energy and energy band gaps of absorption of CH_3OH and C_2H_5OH in SWNT. When exposed to methanol and ethanol, the SWNT-based sensors showed oxidation of products consisting of CH_3O and C_2H_5O. They are calculated with MC and LD simulation methods at different temperatures. All calculations are carried out using Hyperchem7.0 program package.

1. Introduction

Ethanol is the most popular member of alcohol family because of a rare blend of its useful and harmful effects. This is the only alcohol which most of people, all over the world, encounter in their daily life. Detection and control of alcohol is necessary, especially when we are speaking about people's behavior in society. Ethanol sensors can have applications in different areas, such as control of drunk-driving and monitoring of fermentation and other processes in chemical industries. Development of ethanol sensors based on thin film technology offers the advantages of greater sensitivity, shorter response time and lower costs, among these sensors SWNTs are the latest ones which are in use today.

A SWNT can be metallic, semi-conducting, or semi-metallic, depending on its chirality [1]. Utilization of these properties has led to applications of individual nanotubes or ensembles of nanotubes as scanning probes [2,3], electron field emission sources [4], actuators [5], and nano-electronic devices [6]. Here, we report the realization of individual semi-conducting-SWNT (S-SWNT)-based chemical sensors capable of detecting small concentrations of alcohol gas molecules.

SWNTs can be chiral or nonchiral, again depending on the way of the rolling up vector, $C = na_1 + ma_2 = (n, m)$, where a_1 and a_2 are the primitive lattice vectors of the graphene and n and m are integers [7,8]. SWNTs are classified into three types namely, armchair (n,n) nanotubes, zigzag (n,0) nanotubes, and chiral (n,m) nanotubes with $n \neq m$ (Fig. 1) [9]. SWNTs are metals when $(n-m)/3$ is an integer, otherwise they are semiconductors [10]. The tubes are uniquely characterized by a pair of integers (n,m) that are components of the vector defining the direction in which the graphite sheet was rolled up (e.g. Fig. 2).

Chemical sensors based on individual SWNTs are demonstrated in Fig. 2. Exposing to gas molecules such as C_2H_5OH and CH_3OH, the electrical resistance of a semi-conducting SWNT is found to dramatically increase or decrease. This serves as the base for nanotube molecular sensors which is shown in Fig. 3. The nanotube sensors exhibit a fast response and a substantially higher sensitivity than that of existing solid-state sensors at room temperature. Sensor reversibility is achieved by slow recovery under environmental conditions or by heating to high temperatures.

In previous reported alcohol vapor sensors based on SWNT field effect transistors (FETs), the structure of the FET sensor and the experimental geometric response are schematically shown in

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doi:10.1016/j.mejo.2010.01.011

Fig. 3 [11]. The interactions between molecular species and SWNTs and the mechanisms of molecular sensing with nanotube molecular wires are investigated. The SWNTs can cover the surface of metal (Pt) wire and stay in horizontal or vertical position (part (B), Fig. 3). The alcohol molecules may pass through SWNT, when SWNTs are horizontal (Fig. 4) or they may oxidized to CH_2O and C_2H_4O, when they are vertical on Pt (Fig. 5).

All the geometric optimized structures were carried out using Gaussian program package. Density functional theory (DFT) was used in optimized intermediates and transient states of them. Nowadays, first-principles methodologies based on Monte Carlo (MC) and Langevin dynamics (LD) simulations can provide precise calculations of the total energetic and potential energy of the adsorption. There are three steps in carrying out any quantum mechanical calculation in Hyperchem7.0 program package [12]. Hyperchem uses the Metropolis method [13], which chooses

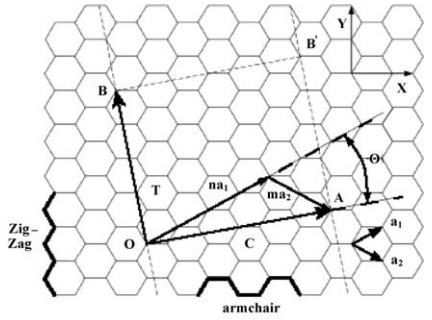

Fig. 1. Schematics of the generation of a carbon nanotube by folding a section of graphene sheet.

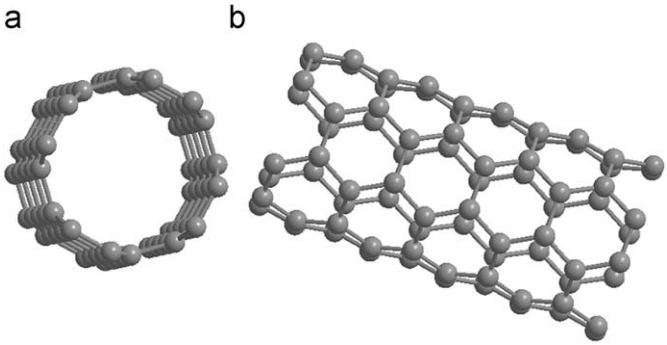

Fig. 2. Optimized configuration: (a) top-view and (b) side-view SWCNT (4, 4).

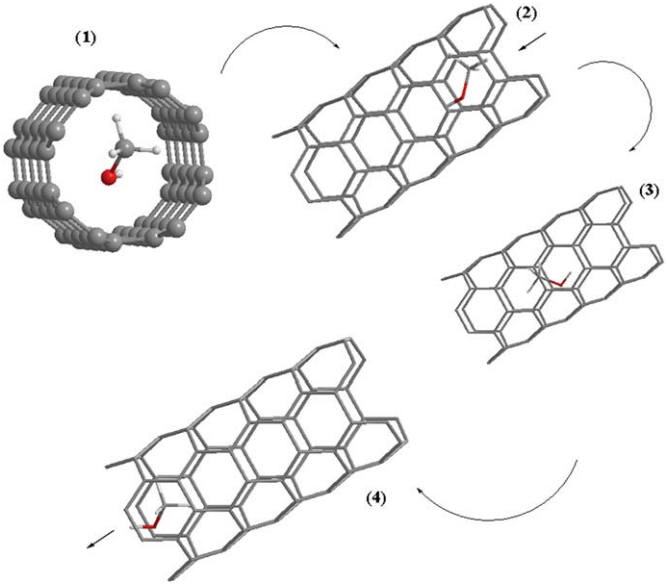

Fig. 4. Configuration top-view and side-view of CH_3OH passing through SWNT length.

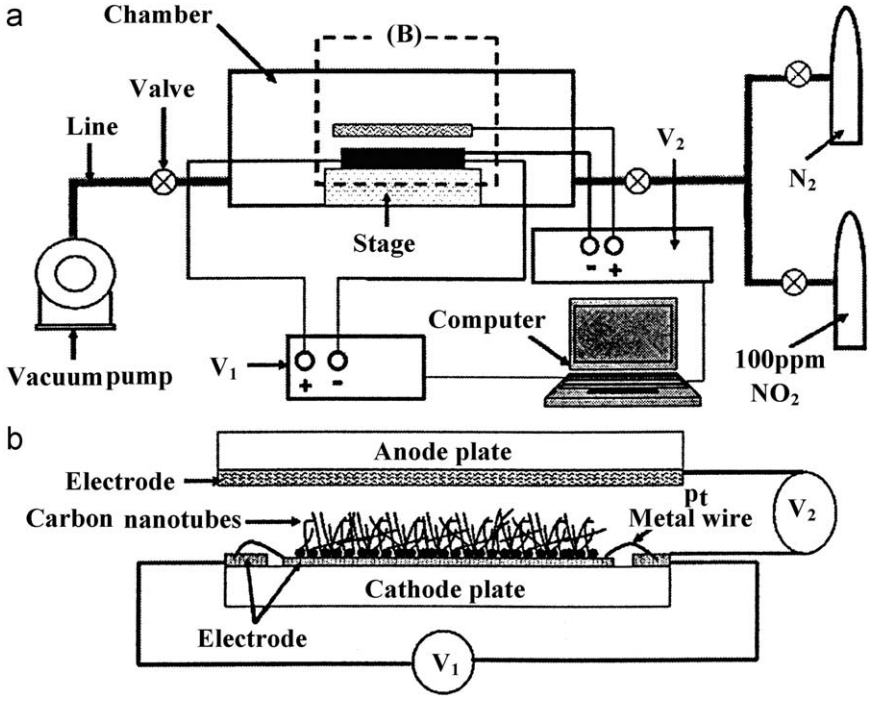

Fig. 3. Cross sectional structure of the SWNT field effect transistors (FET-based sensor) and the experimental geometry [11].