Nano Temperature Sensor Based on the Adaptive Intermolecular Reactive Bond Order Potential Model

Ahmad Al Badawi [1] **and Qasem Abu Al-Haija** [2]

[1] Department of Computer Engineering, Taif University, Al-Taif, 21974, P.O. Box 888, Saudi Arabia
[2] Department of Electrical Engineering, King Faisal University, Al-Ahsa, 31982, P.O. Box 380, Saudi Arabia

Abstract: A nano temperature sensor is proposed here based on the Adaptive Intermolecular Reactive Bond Order (AIREBO) potential to detect the temperature of the surrounding ambient. By calculating the potential energy of covalent bonds using AIREBO model, the relation between the applied temperature on carbon nanotubes and the AIREBO potential for the single covalent bond (C–C) can be found. This work is simulated by Nano-Hive simulation tool in addition to HiveKeeper which provides a visual displaying of the simulation results produced from the Nano-Hive.
Keywords: Nano-Sensor; Carbon nanotubes; AIREBO; Nano-Hive.

1. Introduction

A nanometer (nm) is one thousand millionth of a meter. For comparison, a single human hair is about 80,000 nm wide, a red blood cell is approximately 7,000 nm wide and a water is about 0.3 nm across. Nanotechnology means: the manipulation and manufacturing of materials and devices on the scale of atoms or small groups of atoms. More specifically, the manipulation and manufacturing of materials within range 100 (nm) [1].

Nanotechnology is not a new notion, its roots belongs to the physicist Richard Feynman when he presented a lecture under the title "There's Plenty of Room at the Bottom" [3] in 1959. He described how the 24 volumes of Britannica encyclopedia could be written on the head of a pin. This lecture was the trigger which struke the world and made scientists tend to nano scale. Carbon nanotubes [9], which discovered 1991 by Sumio Iijima [4], are known to be the basic material for nanotechnology due to their extraordinary characteristics such as thermal conductivity and mechanical and electrical properties. In this study, Single-walled Carbon Nanotube (SWNT) is used to sense the ambient temperature throught (AIREBO) potential model. AIREBO is an enhanced version of reactive empirical bond-order (REBO) model which is a function for calculating the potential energy of covelant bonds. REBO states that the expression of the total potential energy of a system is the sum of nearest-neighbor pair interactions which depend on the coordination of atoms and their local atomic environment [7]. D. Nakabayashi et. al. [13] have reported the generation of reinforced carbon−carbon composite nanotools using a nanotube (CNTs) covered by an amorphous carbon matrix (shell); the CNT tip protruded and remained uncoated to preserve apex size. They have shown that Unsuitable properties such as flexibility and vibration could be controlled without deteriorating the CNT size, strength, and resilience as well as run many nano-manipulation experiments and molecular dynamics simulations to study the mechanical response of these composite beams under bending efforts.

Sensing is certainly a quality that we associate with living being. A stone does not sense, but can a silicon circuit do it? Of course, the answer is yes. "Sensors are devices that detect or measure physical and chemical quantities such as temperature, pressure, sound, and concentration. The measurands are converted into an electrical signal" [8, 10, 11]. Nano-sensors can lead to many advantages such as low weight, low power consumption, high density deployment, and maybe low cost. Nano-sensor is not a new device; they had been constructed using silicon via Micro Eletro-Mechanical (MEM) technology [6]. Now, nano-sensors can be constructed using CNT [5].

This work is motivated by the potential of employing nanotechnology in Wireless Sensor Networks (WSNs) to construct a whole nano wireless sensor node. A nano wireless sensor node can be constructed by implementing individually each component of the sensor node at the nanoscale, and then assembling these components with each other to get a whole nano wireless sensor node. By minimizing all function units to the nanoscale, many problems associated with current WSNs can be resolved. Not to mention, the various characteristics of CNT will enhance the performance of node. The purpose of this work is to propose a nano-sensing unit by exploiting AIREBO potential model to estimate the ambient temperature.

2. System Equations

As we have said, AIREBO model is used to find the potential between (C–C) covalent in SWNT. This potential can be described as follows [12]: The general form of this potential, originally is derived by Abell from chemical pseudopotential theory, is described in Equation1:

$$E_b = \sum_i \sum_{j>i} \left[V^R(r_{ij}) - b_{ij} V^A(r_{ij}) \right] \quad \text{..... 1}$$

Where:

- $\mathbf{E_b}$ is the chemical binding energy
- **i, j** are nearest neighbor atoms
- $\mathbf{r}_{ij}$ is the distance between atoms i and j
- $\mathbf{V}^R$ is the interatomic, pair-additive repulsive function (core-core, etc)
- $\mathbf{V}^A$ is the interatomic, pair-additive attractive function (from valence electrons, etc)
- $\mathbf{b}_{ij}$ is a bond order between atoms i and j

AIREBO also uses the Van Gunstern-Berendsen Thermostat which controls the thermal activity of the system. The formula of this Van Gunstern-Berendsen Thermostat is described in [12] as follows:

$$\lambda = \left[1 + \frac{\triangle t}{\tau_T} \left\{ \frac{T_0}{T\left(t - \frac{1}{2}\triangle t \right)} - 1 \right\} \right]^{\frac{1}{2}} \quad \text{.....2}$$

Where:

- $\boldsymbol{\lambda}$ is the temperature scaling factor
- $\boldsymbol{\Delta t}$ is the time step (time between iterations)
- $\boldsymbol{\tau_T}$ is a time constant
- $\mathbf{T_0}$ is the environment (bath) temperature
- $\mathbf{T(t\text{-}1/2\Delta t)}$ is the temperature half time step ago

AIREBO treats with each atom as an individual entity that has its position, velocity, and acceleration. These parameters are used to calculate the kinetic energy. In this work we examine the effect of ambient temperature on a SWNT consists of 104-carbon-atom with 148 single-covalent bonds. The AIREBO potential is calculated with different temperature values.

3. Simulation Environment

Nano-Hive is a modular simulator used for modeling the physical world at a nanometer scale. This tool can be used in order to examine the performance of the systems that constructed at nanoscale. Nano-Hive can give an indication about the stability of the system at nanoscale. Stability is so important in nanotechnology as systems are built atom by atom, and as we know, there are many factors which have a great effect on atoms such as the interaction between atoms and the forces between atoms. All these factors must be explored in prior to the manufacturing stage.

HiveKeeper is another tool used in this work to provide a visual display of the simulation which produced from Nano-Hive. Nano-Hive is introduced for two types of computational situations: a desk-top version for very simple molecular systems, and fully distributable and parallel versions for larger simulations. The distributable or parallel versions could run on stand-alone networks. In this work, we use a single desk-top version. Nano-Hive incorporates many plug-ins for key simulation functions. These plug-ins look like the functions in conventional programs. The following plug-ins are used in this work:

- The Entity Management plug-in which is responsible for storing all simulation data including atoms, bonds and molecules.
- The Physical Interaction plug-in which performs the actual calculations that model the world at nanometer scale.
- The RC-Traverser plug-in which provides to each physical interaction plug-in the entire system for simulation.
- AIREBO plug-in performs reactive molecular dynamics for hydrocarbon systems.
- The Simulation Results plug-ins are invoked to provide results of the simulation.

4. Proposed Implementation

In order to build a program that can be run on Nano-Hive we have to specify the following files:

- The configs.txt file which specifies the configurations of the simulator such as adding or removing plug-ins and desk-top or distributed version. We have used the default file which installed with the simulator.
- The input.nml file which acts as input data. These data are used to describe atoms coordination.
- The simulation-specification.xml file which specifies the simulation conditions such as input files, traverser plug-ins, result plug-ins, and output files.
- The simulation-workflow.tcl file is a TCL script that tells Nano-Hive how to process the simulation. The same script can be used for many different simulations.
- The results.txt file which used as a host for the results of the simulation.
- The results folder which used to host the files needed by Hivekeeper to display the simulation graphically.

We will thoroughly demonstrate these files in the following sub-sections.

4.1 The Input File

In this file the coordination of the 104 carbon atoms is specified as well as single covalent bonds between carbon atoms. Our SWNT is irregular polygon of order (8). The design of the SWNT is given below in figure 1. The previous figure shows the design of our SWNT. These two designs are repeated 6.5 times to get 104-atom and 148 (C–C) bonds. This arrangement of atoms considered as the input of our simulation. All the dimensions are in nm.

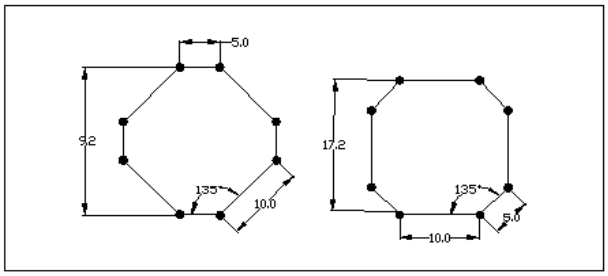

Fig. 1 The front projection of the SWNT.

4.2 The Simulation Specifications File

This file contains the specifications of the simulation such as the number of iterations, the time between iterations, and the plug-ins parameters.

In our work the following specifications are used:

- The start iteration variable = 0.
- The iterations value = 1000.
- Environment temperature used as a parameter for the temperature, we use 300K temperature in our work.
- The time between iterations is set to 5e-16. Less than this value, the system will be unstable.
- The plug-ins parameters are also defined here.
- The results.txt file and the results folder are also specified here.

AIREBO plug-in has one parameter named as (deltaTbyTau). This parameter refers to the ($\Delta t/\tau T$) term in the Van Gunstern-Berendsen Thermostat used by the plug-in. The range is [$0.01 < \Delta t/\tau T < 1.2$] where 1.2 greatly dampens any thermal activity in the system, and 0.01 barely dampens thermal activity [12]. In this work we chose ($\Delta t/\tau T = .4$) which provides the best results.

4.3 The Simulation Workflow File

This file acts as the context of the simulation, i.e how to process the input. This file is so similar to the workflow file in cnt55 example which is included in the simulator itself. The function of this file can be summarized as follows:

- The simulator imports the input file.
- A loop of predefined number of iterations is invoked.
- In this loop the simulation is prepared and then the input is applied on AIREBO plug-in to do the needed calculations.
- Finally, the results are sent to the result plug-in.

5. Simulation Results

The simulation results can be extracted from the (results.txt) file. This file contains the following data:

- Iteration number.
- Time stamps which refer to the starting time of the associated iteration.
- Ideal temperature in Kelvin. The simulator alters the temperature every iteration.
- Kinetic energy in joule calculated using AIREBO plug-in.
- Potential energy in joule calculated using AIREBO plug-in.
- The total energy which implement the summation of the kinetic energy and the potential energy calculated using AIREBO plug-in.

The following table contains the portion of the simulation results, the kinetic energy, the potential energy, and the total energy.

Table 1. Simulation Results.

Iteration Number	Temperature in Kelvin	Total Energy * e-19	Potential Energy * e-19	Kinetic Energy * e-19
20	3236.9	-792	-931	139
40	926.8	-943	-983	39.9
160	336.8	-1147.3	-1161.8	14.5
180	318.6	-1151.7	-1165.4	13.73
860	310.7	-1148.5	-1161.88	13.4
200	303.7	-1153.3	-1166.4	13.08
700	300.1	-1147.1	-1160.1	12.93
740	298.1	-1148.2	-1161.0	12.84
800	293.9	-1143.8	-1156.5	12.66
940	283.6	-1148.0	-1160.2	12.22

960 0	278.2 0	-1144.5 0	-1156.5 0	11.986 0

According to the data in this table, we can extract the following figures:

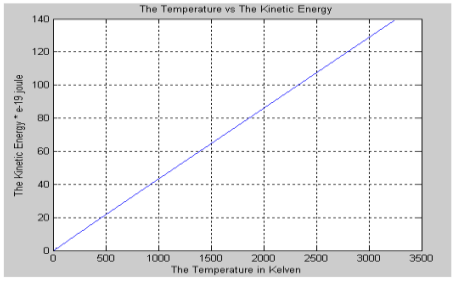

Fig. 2 The Kinetic Energy vs. Temperature.

As we can see in the figure, the kinetic energy acts as a linear function with respect to the applied temperature. We can describe this function as follows:

$$K = a * T \quad \ldots\ldots \textbf{(3)}$$

Where (a) is the gradient.

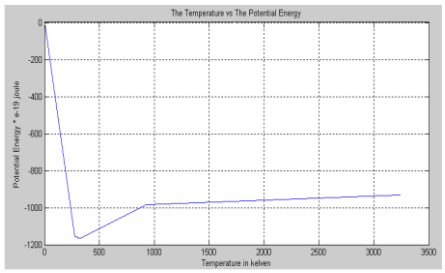

Fig. 3 The Potential Energy vs. Temperature.

As we can see in figure 3, the potential energy does not act as the kinetic energy with respect to the applied temperature. Potential energy changes dramatically with respect to the change of ambient temperature especially when it is less than 500 K. This forms the basis of our nano-sensor. If we can calculate this potential energy in SWNT incorporated within the nano-sensor, the ambient temperature can be easily found.

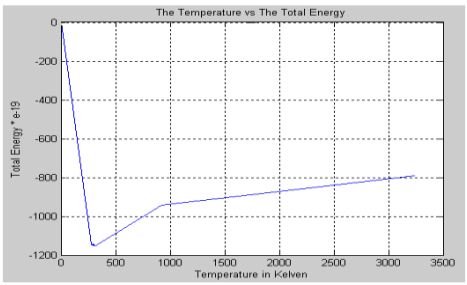

Fig. 4 The Total Energy vs. The Temperature.

Figure 4 shows the relation between temperature and total energy. The total energy can be used to sense the ambient temperature but it requires more consumption and power consumption which is one of the main drawbacks in current sensor nodes.

6. Conclusions

Unfortunately, this system requires a high level of data processing since the collected data are of small values. However, this model is so accurate that it can detect a tiny change in the temperature of the surrounding environment (this can be noticed from table 1). Also this system is stable at any temperature due to the properties of the SWNT, which makes this system applicable at any temperature and for any application. As we have said, the stability of the system can be noticed via HiveKeeper. This model can be modified by many ways. One of them is to doping the SWNT by some elements like H, Cl, and F. Or by plunging it in gases like O2, CO2, broban or methane. These methods can only be evaluated by trial and fault principle in order to decide system efficiency. This model can also be modified in order to sense the pressure or the humidity of the surrounding environment to attain a whole sensing unit that can be exploited not only in WSN but also in many other applications.

References

1. Drexler, K. Eric, “Engines of Creation: The Coming Era of Nanotechnology”. Doubleday, 1986.
2. Shin-Lin Wu and Yu-Chee Tseng, "Wirelees Ad Hoc Networking Personal-Area, Local-Area, and the Sensory-Area Networks" Ebook. Ch. 2 Communication protocols. Page 26.
3. Michael Roukes, "Scientific American Reports Special Edition on Nanotechnology". Magazine. Published by the staff of Scientific American, September 2007. Page 4.
4. Linda Williams and Dr. Wade Adams, "Nanotechnology Demystified A Self-Teaching Guide". Ebook. 2007. Ch 1. Pages 11,12.
5. Niraj Sinha, Jiazhi Ma, and John T. W. Yeow, "Carbon Nanotube-Based Sensors". Journal of Nanoscience and Nanotechnology Vol.6, 573-590, 2006.
6. Franck CHOLLET and Haobing LIU, "A (not so) Short introduction to MEMS ", version 2.0, Aug 2006. Ch 2 Page 19.
7. S. J. Stuart, A. B. Tutein, and J. A. Harrison, “A Reactive Potential for Hydrocarbons with Intermolecular Interactions”, Journal of Chemical Physics. 112, 6472 (2000).

8. P. J. Burke, Member, IEEE, S. Li, Member, IEEE, and Z. Yu, Member, IEEE, "Quantitative Theory of Nanowire and Nanotube Antenna Performance", Nanotechnology, IEEE Transactions on Volume 5, Issue 4, July 2006 Page(s): 314 - 334.
9. Mike Foley, "Carbon Nanotubes 101 A practical guide to understanding their properties, applications, production methods, markets and utility". March 1st, 2006. http://www.nanotech-now.com/Carbon-Nanotubes-101.htm
10. N.P Mahalik, "Micromanufacturing and Nanotechnology". Springer-Verlag Berlin Heidelberg 2006.
11. American Association For The Advancement Of Science, "Nano-Transistor Switches With Just One Electron, May Be Ideal For Molecular Computers, Science Study Shows", ScienceDaily (Jul. 9, 2001). http://www.sciencedaily.com/releases/2001/07/010709073509.htm
12. Nano-Hive Version 1.2.0 Beta 1 documentation.
13. D. Nakabayashi et. al., " Carbon Nanotubes as Reinforcement Elements of Composite Nanotools", Nano Lett., 2008, 8 (3), pp 842–847