Behavior Analysis and Optimization of Zinc Oxide (ZnO) Nanowire using Molecular Dynamic Simulation

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Abstract— Nanowires are the structures which have a diameter limited to less than ten nanometers and an unlimited longitudinal length. The syntheses, characterization and analysis of Zinc Oxide (ZnO) nanowire of hexagonal form have practically carried out using chemical deposition method. There are numerous practical analysis and characterization methods for nanowires such as spectrophotometer, scan electron microscope, energy dispersive X-ray study and X-ray diffraction. In this paper, a theoretical analysis and characterization of nanowires are presented. This paper mainly estimates the behavior analysis and optimization of Zinc Oxide (ZnO) nanowires using molecular dynamic simulation with the help of MATLAB. Finally, the result of molecular dynamic simulation for Zinc Oxide (ZnO) nanowire is compared with carbon nanotubes.

Keywords— Nanowire, Zinc Oxide, Stability Optimization, Simulation.

I. INTRODUCTION

The nanowire is basically a nanostructure, having diameter in the range of 10^{−9} meters. At these level, the value of quantum mechanics is significant and originated the term quantum wires [1]. There are different types of nanowires available, like metallic (Ni, Au, Pt), semiconducting (GaN, Si, InP, ZnO) and insulating (SiO_{2}, TiO_{2}) [1]. Generally, nanowires have length-to-width ratio around 1000 and it is referred to as the one-dimensional materials. The characteristics of nanowires have many interesting which are not in the bulk materials, because electrons in the nanowires are quantum enclosed and dominate energy levels which are different from traditional energy bands of bulk materials [2]. The superior features of this quantum enclosed revealed by particular nanowires basically represented as discrete values of the electrical conductance [3]. Such distinct discrete values originated from a quantum mechanical limitation on the number of electrons which can travel throughout the wire at nanometer scale.

ZnO is a representative II-VI semiconductor material within a wide band-gap of 3.37 eV at normal room temperature [4]. Even though its value of band-gap is nearer to GaN (3.44 eV), its exciton molecular binding energy is 39 eV, that is higher and sophisticated as compared to GaN (25 meV) [5][6]. Theoretically, gathering of high efficient UV exciton emission and laser at normal room temperature propose the applications of UV laser in the fields of detection, communication and optical memory with magnitude enhancement and performance was achievable [4][5]. The melting point of ZnO is 1954°C, this determines high thermal and chemical stability. Again, ZnO has potentials due to its affordability, abundant in nature, environmentally, eco-friendly, simple fabrication processes and some others [3]. Various physicochemical and electrochemical deposition techniques have been reported to create oriented metal oxide semiconductor nanowires [5]. Techniques like catalytic progress through vapor-liquid-solid epitaxial methods, metal-organic chemical vapor deposition, pulsed laser deposition, chemical vapor deposition, hydrothermal synthesis, chemical solution approaches and chemical electrode position have been particularly successful in creating sensitive oriented arrays of anisotropic nanowires of ZnO [12][13].

In general, there are two separate approaches for creating nanowires: top-down and bottom-up strategies [13]. The top-down approach basically including etching and lithography technique in bulk materials for structuring functional devices, this method has been effective in many locations [16]. In the bottom-up method, purposeful nanostructures are gathered from well-defined chemically and physically synthesized building blocks. Zinc oxide (ZnO) nanowires are commonly synthesized using a bottom-up approach [17].

II. LITERATURE REVIEW

In this paper we reviewed, explored and analyzed some molecular dynamic simulation of some nanowires of different materials.

A. Molecular Dynamics Simulation Study of Carbon Nanotubes

Molecular dynamics simulation [14] has been used extensively to explore the behavior of nano-oscillators. In this study and analysis, damped oscillating behavior between the centers of inner mass and outer nanotube of double-walled carbon nanotube by using molecular dynamics simulation was presented. Other analysis investigated the oscillatory behavior of a double-
walled boron nitride nanotubes [14]. It presents that boron nitride nanotube oscillators have higher frequency than the carbon nanotubes oscillators. Some experimental results have investigated the effects of the radius and defect of a single-walled carbon nanotubes on oscillating behavior of C60 which oscillates inside the single-walled carbon nanotubes by using molecular dynamics simulation [14]. The couple oscillation of multi-walled carbon nanotubes oscillators shows that the frequencies of the multi-walled carbon nanotubes oscillators are higher than those of the double-walled carbon nanotubes oscillators. Nowadays, it refers to some applications of MATLAB for calculating the power spectral and spectrogram of a fullerene oscillating as a nano-oscillator inside a carbon nanotube.

Current achievements in nanotechnology are capable to produce technologies which exploit nano-devices with novel and fundamentally unique properties. The high proficiency of these devices has produced a significant interest over the recent years in numerous theoretical and experimental exploration groups so that designing this type of nano-devices and their applications have become a specific area in nanoscience and nanotechnology. Zinc Oxide (ZnO) and fullerenes are two significant types of nanostructures, which have exclusive mechanical, physical, and chemical properties. These unusual properties of nanostructures promise innovative nano-devices based on Zinc Oxide (ZnO) and fullerenes.

B. Molecular Dynamics Simulation of Oscillatory Behavior of Fullerene Inside Carbon Nanotubes

It achieved molecular dynamics simulation for an oscillating fullerene C60 inside a single-walled carbon nanotubes and also inside a nanotube bundle, distinctly [15]. The force field and Van Der Waals force potential function as non-bonding interaction is applied in this simulation. It uses a canonical ensemble and the Nose–Hoover thermostat algorithm. The Beeman integration scheme is used with a time step size of 1.0 fs. The cut-off distance is 12.5 Å and the temperature was fixed at 100 K. Figures 1 and 2 represents two snapshots of fullerene C60 oscillating inside carbon nanotubes (15, 15) and nanotube bundle (10, 10), respectively.

It has been presented that carbon nanotubes in their different forms, including single-walled carbon nanotubes, double-walled carbon nanotubes, multi-walled carbon nanotubes, carbon nanotubes bundle, and also fullerenes oscillating inside a nanotube such as a single-walled carbon nanotube, which can be considered as nano-oscillators. Outcomes of recent studies have directed researchers to conclude that these oscillators are capable to produce high frequencies, primarily in the gigahertz range [15]. The beneficial applications of these gigahertz oscillators have been of value to various researchers, particularly electrical engineers [15].

The nano-oscillators were first introduced by presenting that sliding of inner shell inside the outer shell of a multi-walled carbon nanotubes can generate oscillatory frequency up to some gigahertzes [17]. It demonstrated the controlled and reversible telescopic extension of multi-walled carbon nanotubes. Repeated extension and retraction of telescoping nanotube segments exposed no wear or fatigue on the atomic scale, these nanotubes constitute near perfect, wear-free surfaces. There have been conventional applied mathematical investigations into the mechanics of nano-oscillators, which have been done primarily by analysis of the oscillators involving atoms, spherical and spheroidal fullerenes, and carbon nanotubes.
oscillating in a single-walled, double-walled, and multi-walled carbon nanotubes [18]. Also various experimental analysis regarding the interesting field of nano-oscillators and molecular dynamics simulations have discovered some innovative characteristics of them.

III. PROPOSED METHOD

Zinc Oxide (ZnO) nanowire nano-structures and summarize the essential mechanics of the gigahertz nano-oscillators. The method introduces a potential for the non-bonded interaction energy between two molecules. By using this approach, it determines the interaction energies of a fullerene situated inside a bundle. From the potential energies, the Van der Waals restoring forces are obtained, which are applied to estimate the oscillatory behaviors of nano-oscillators. The non-bonded interaction energy \( W \) is obtained by summing the interaction energy for each atomic pair,

\[
E = \sum_i \sum_j \Phi(r_{ij}),
\]

where \( \Phi(r_{ij}) \) is a potential function for atoms \( i \) and \( j \) at distance \( r_{ij} \) apart. In the continuum approximation, it is expected that carbon atoms are uniformly dispersed over the surface of the molecules. Therefore, the double summation in the above equation can be replaced by a double integral, which averages over the surfaces of each entity.

\[
E = n_1 n_2 \int \int \Phi(r) \, d\Sigma_1 \, d\Sigma_2
\]

Where, \( n_1 \) and \( n_2 \) are the mean surface density of atoms on each molecule \( r \) is the distance between two typical surface elements \( d\Sigma_1 \) and \( d\Sigma_2 \) on each molecule. There are a number of models of potential for \( \Phi(r) \) with the following equation:

\[
\phi(r) = \frac{A}{r^6} + \frac{B}{r^{12}}
\]

Where \( A \) and \( B \) are the attractive and the repulsive constants, respectively, \( r \) is the distance between two atoms, the above equation can be written as:

\[
\phi(r) = 4\varepsilon \left[ \left( \frac{A}{r} \right)^6 + \left( \frac{B}{r} \right)^{12} \right]
\]

where \( \sigma \) and \( \varepsilon \) are the Van der Waals diameter and the respectable depth, \( \varepsilon = A2/(4B) \). The equilibrium distance \( r_0 \) is given as:

\[
r_0 = 2^{1/6} \sigma = \left( \frac{2B}{A} \right)^{1/6}
\]

The total interaction energy of the fullerene radius \( r_0 \) located at the center of a bundle containing \( N \) Zinc Oxide (ZnO) nanotubes of infinite length is given by:

\[
W = -N E(R)
\]

Where, \( R \) is the bundle radius, is the distance from the center of the fullerene to the axis of the nanotubes in the bundle \( E \) is the interaction energy between the fullerene and a single Zinc Oxide (ZnO) nanotubes.

\[
E(R) = 4\pi r_0^2 \eta_f \eta_t \left[ \frac{B}{256} r_0^6 \sum_j \left( \frac{1155}{128} r_0^6 J_6 + \frac{9009}{256} r_0^6 J_7 \right) \right]
\]

Where \( \eta_f \) and \( \eta_t \) are the mean atomic densities of the fullerene and Zinc Oxide (ZnO) nanotubes, respectively \( J_n \) is defined in terms of hypergeometric function as:

\[
J_n = \frac{2\pi}{(r - R)^2 - r_0^2} \eta_t \eta_f \left[ F \left( \frac{1}{2}, n \right) + \frac{1}{2} ; 1; \frac{r_0^2}{(r - R)^2} \right]
\]

The parameters of total energy for Zinc Oxide (ZnO) nanotubes bundle are:

\[
\eta_f = 0 \ldots .3789 \text{ Å}^{-2} \eta_t = 0.3812 \text{ Å}^{-2} \varepsilon = 41 \text{ eV} B = 22534 \text{ Å}^{-2} A = 6 \ldots .\text{ Å}12
\]

The velocity of the oscillating fullerene inside a Zinc Oxide (ZnO) nanotubes bundle is given by:

\[
\nu = \left[ \frac{2W}{M + \nu_0^2} \right]^{1/2}
\]

Where \( M \) is the mass of the fullerene which is equal to \( 1195.2 \times 10^{-27} \text{ kg} \). \( \nu_0 \) denotes the initial velocity of the fullerene, which here is assumed to be zero. Also the oscillatory frequency \( f \) is determined from:

\[
f = \frac{\nu}{(4L)}
\]

IV. SIMULATION AND RESULT EVALUATION

As a simulator, we used MATLAB for our implementation and performance evaluation of our proposed method. The radial distribution function analysis curve obtained for Zinc Oxide (ZnO) and carbon nanotubes is shown in figure 3, which
represents the behavior analysis and optimization of zinc oxide (ZnO) nanowire using molecular dynamic simulation.

Molecular dynamics simulations were performed using the force field. The force field has been measured to calculate the structures and energies, conformational energies, including heats of formation and rotational barriers for Zinc Oxide (ZnO) nanotubes more accurately as possible with previous force fields.

The total potential energy ($E_{\text{total}}$) of this simulated systems is calculated as the sum of the eight individual energy terms including

$$E_{\text{total}} = E_s + E_\theta + E_{\omega_s} + E_{\omega_\theta} + E_{\omega_b} + E_{\theta\theta} + E_{\text{vdw}}$$

where $E_s$, $E_\theta$, $E_{\omega_s}$, $E_{\omega_\theta}$, $E_{\omega_b}$, $E_{\theta\theta}$, and $E_{\text{vdw}}$ are the energies corresponding to bond stretching, angle bending, torsion, stretch-bend interaction, torsion-stretch interaction, torsion-bend interaction, and van der Waals interaction terms, respectively. With the help of radial function analysis in the simulation result, it is concluded that Zinc Oxide (ZnO) nanowires performs better as compared to carbon based nanowires.

### V. CONCLUSION

Results represents that the behavior analysis and optimization of Zinc Oxide (ZnO) nanowire using molecular dynamic simulation process, which is very sensitive to the applied parameters which consequences better as compared to carbon nanotubes. This results approve this fact in a compatible way together. The works exposed that nanotube curvature may directly affect the single-walled Zinc Oxide (ZnO) nanowire adsorbate atomic potentials, which is the subject of future research based on the intermolecular potentials obtained from quantum chemical calculations.

### REFERENCES


