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Numerical Modeling and Heuristic Algorithms for Nanogenerator Behavior Analysis

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Abstract— **Recently, the desire for a self-powered micro and nanodevices has attracted a great interest of using sustainable energy sources. Further, the ultimate goal of nanogenerator is to harvest energy from the ambient environment in which a self powered device based on these generators is needed. With the development of nanogenerator-based circuits design and optimization, the building of new device simulator is necessary for the study and the synthesis of electromecanical parameters of this type of models. In the present article, both numerical modeling and optimization of piezoelectric nanogenerator based on zinc oxide have been carried out. They aim to improve the electromecanical performances, robustness, and synthesis process for nanogenerator. The proposed model has been developed for a systematic study of the nanowire morphology parameters in stretching mode. In addition, heuristic optimization technique, namely, particle swarm optimization has been implemented for an analytic modeling and an optimization of nanogenerator-based process in stretching mode. Moreover, the obtained results have been tested and compared with conventional model where a good agreement has been obtained for excitation mode. The developed nanogenerator model can be generalized, extended and integrated into simulators devices to study nanogenerator-based circuits.**

Keywords— Numerical modeling, Heuristic Algorithms, Nanogenerator, Particle Swarm Optimization, Electrical potential

I. Introduction

Nowadays the extensive use of micro and nanodevices in different fields such as making energy from the operating environment is increasingly rising. In particular, for nanogenerator, the energy can be harvested from various sources as incident chocks, mechanical vibrations, radiofrequency waves, and fluids flows to ensure self-powered devices [1-4]. Especially, mechanical energy is available almost everywhere and consequently exploited in our daily life [5-8]. Few decades ago, the evolution in micro and nanotechnology has allowed the researchers to manufacture miniature devices able to convert mechanical energy into electrical one [9]. It is especially possible for applications in biomedical devices, sensors and computing to stretch out their capability by removing the batteries and power cables [10-14]. Accordingly, piezoelectric materials (ZnO) with a crystal structure have been practically used to make up energy harvesting devices. Hence, these materials can be considered as reliable high performance sources due to their non-toxicity and cost effectiveness [3].

Taken into account the ability of converting the ambient mechanical energy into electrical potential by piezoelectric nanogenerator (NG), serious developments of these NG devices have been investigated. For instance, Wang et Al. [9] have successfully developed a piezoelectric nanostructure that can power a light-emitting diode (LED) by applying a strain on the nanostructure. However, the main disadvantage of this NG is power time limitation. Other realized circuits include different electronic components such as rectifiers, voltage amplifiers, integrated circuits and inductors [5]. Since the contributions in the NG-based circuits' investigations detected some problems in terms of efficiency, number of additional components, and difficulty of implantation, a simulator devices based study is then necessary before implantation of these circuits [6].

In this article, numerical modeling and optimization of Zinc Oxide (ZnO) piezoelectric nanowires (NWs) are carried out to improve electromecanical performances, robustness, and synthesis process for NG. The numerical model has been developed for a systematic study of the NWs morphology parameters in stretch mode. In this context, a mechanical equation that links stress to applied external forces was coupled with piezoelectricity equations and the whole system is solved by finite element method (FEM) [11][15]. The NW is modeled as a cylinder where its bottom and upper parts are fixed in order to apply the external force. In addition, heuristic optimization technique, namely, particle swarm optimization (PSO) has been employed in order to transform modeling problem into optimization one. The database used for the optimization of our analytic NWs model is built on the numerical model of the NWs based on ZNO material.

The remainder of this article is organized as follows: in the following section, the numerical model of NG based on ZnO materials is established and its analytic model is then determined and optimized using PSO algorithm. Section three exhibits the results of our approach. The last section summarizes our contribution and states remarks and comments for future work.

II. Modeling and Methodology

The nanogenerator consists of a set of nanowires that lies between two gold electrodes on two opposite substrates. Fig.1. The surface of the substrate is $1cm^2$ in silicon material. This latter is floppy and adaptable to future self-powered nano or microdevices. The substrate is used to

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calculate the strain distribution according to the applied external force, where the functional element of this structure

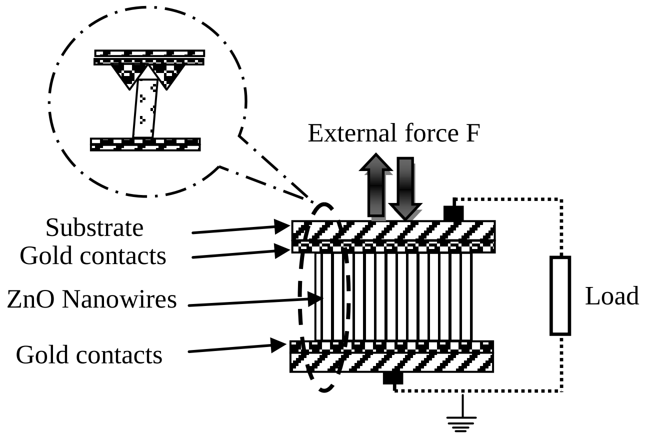

Figure 1. 2D Cross section of nanogenerator.

is the piezoelectric ZnO nanowires. Also, the examination of the NG structure under external force effect in case of stretch mode is made. The external force generates a distributed pressure along the substrate.

In excitation case of the structure, the electrical potential generated by the deformation of ZnO NWs is calculated using computational software COMSOL Multiphysics [16] based on FEM. Each NW is modeled as a cylinder of size 600 nm in length and 25 in radius. The upper and the bottom parts of a NW are fixed on the two substrates. The external force is applied on the upper substrate and generates compression or stretch. For the boundary conditions we assume that the NG is without load and a grounded surface element at the bottom.

The constraint T is linked to the external force F applied on the NW by the following mechanical equation:

$$-\nabla.\mathrm{T} = \mathrm{F} \qquad (1)$$

The electric displacement D and the charge density are expressed as follows:

$$-\nabla.\mathrm{D} = \rho_{\mathrm{v}} \qquad (2)$$

We assume that the study remains under the limit of linear approximations [2]. FEM is used to solve these two equations.

These equations were coupled with the piezoelectricity ones:

$$\sigma_p = c_{pq}\varepsilon_q - e_{kp}E_k \qquad (3)$$

$$D_i = e_{iq}\varepsilon_q - k_{ik}E_k \qquad (4)$$

where σ_p is the stress tensor, ε denotes the deformation tensor, c_{pq} is the linear elastic constant, e_{iq} represents the piezoelectric coefficient, k_{ik} is the dielectric constant, e_{kp} refers to the coupling tensor, D_i is the electric displacement and E represents the electric field.

The geometry where the force is applied has an impact on the FEM calculations. Simulation is difficult to express realistically how the force operates the compression or stretch on the NW. The simple simulation method assumes that the force is applied at a point. However, this force is not realistic and presents a non converging solution at this point. For calculating the solution by FEM, we limit the number of points on the mesh. Thus, the result of the NG excitation by a non-physical point force depends on the mesh size. More precisely, the energy conversion by NG is spent through three stages:

- Firstly, the mechanical energy acts in the piezoelectric transfer process.
- Secondly, the conversion of mechanical energy to electrical energy depends on the NW's electromechanical properties.
- Finally, a junction is created between ZnO and the gold substrate. A current will be generated after the threshold voltage of the current-voltage characteristic (I-V characteristic), and a harvest of electric power will be available at the micro-electrode. In this step the NG can supply an external electric circuit.

A. *Problem Mathematical Formulation*

Fig.2. describes the considered electrical circuit including the equivalent model of the NG under study and a certain load. The aim is to determine an explicit model for the NG. It is focused on finding an adequate relationship between the initial potential and internal parameters of the developed NG.

The total potential generated by the NG is given by:

$$V_{Tot} = V_0 - R_i I \qquad (5)$$

where V_0 represents the initial potential, R_i the internal resistance and I the current density, such that the initial potential depends on the size and the number of the NWs, and the external force. Therefore, the internal resistance should be calculated accordingly:

$$R_i = \rho\frac{l}{s} \qquad (6)$$

where ρ is the wire resistivity, l is the wire length and S represents the cross section of the wire. Substituting Eq. (6) into (5) yields to an analytical potential model with five parameters which will be optimized using PSO algorithm.

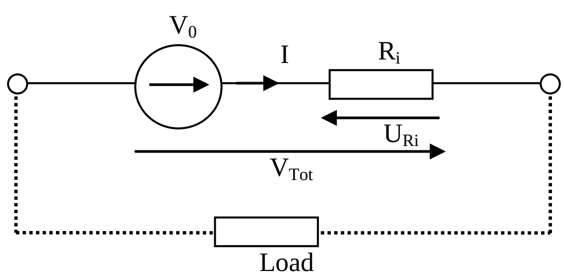

Figure 2. Electrical schema of nanogenerator.

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The aim of this work is to develop an optimal model of NG; this latter is considered as a power source of an electrical circuit where the initial voltage satisfies the features of numerical database. In the NG based model, the relationship between the total voltage and the modeling input parameters can be expressed as:

$$V_{Tot} = f(I, \vec{B}) \quad (9)$$

where I represents the current density, $\vec{B}$ is the parameters vector that will defined in the subsequent discussion and has to be optimized to fit the numerical data base using PSO algorithm [13][17].

The PSO is a population-based approach; its basic principle is formed on the position of each particle in the swarm, where the latter is the potential solution. Such that the particles are flown through a multidimensional search space towards more optimum solutions. Each particle is positioned according to its flying experience and those of its companions. In the swarm, the flying of each particle is influenced by its own speed, the better position that will be achieved and the best known position of the swarm of particles. PSO algorithm is simple and efficient and can be applied to optimize our NG model parameters.

In the developed approach the vector of particles is denoted by $X_k = (F, l, \rho, D, n)$, where the speed and position of each particle in the swarm can be calculated using the following equalities:

$$V_{K+1} = wV_K + c_1 r_1 (p_i - X_K) + c_2 r_2 (p_g - X_K) \quad (10)$$

$$X_{K+1} = X_k + V_{k+1} \quad (11)$$

where c_1 and c_2 are the cognitive and social acceleration factors; r_1, r_2 are random numbers in the range [0,1], X_K represents the position of the particle in swarm, p_i is the local best of the particle, p_g represents the global best of the swarm, and V represents the velocity of particle in swarm [12][18].

TABLE I. Test parameters for the artificial bee colony and particle swarm optimization

PSO parameters	values
Swarm	20
Maximun number of generations	3000
C1,C2	1,1
W	0.9
Obtained fitness value	: 1.1002
Computational time	16.74 min

The fitness function f used for the evaluation of particle swarm is given by:

$$f = \frac{1}{N}\sum\left[\frac{V_{Num,Exp} - V_{Bees\,or\,PSO}}{V_{Num,Exp}}\right]^2 \quad (12)$$

where N is the total number of data base points, the indices "Num" and "PSO" indicate respectively numerical data, calculated data by PSO algorithm. The objective is to minimize the fitness function in order to find the best solution and ensure the precision of the analytical NG voltage model.

III. Results and Discussions

To optimize the proposed formulation (Eq. 12), program for PSO algorithm is developed. For the PSO algorithm configuration, the initial population is taken as 20 particles, where the maximum number of generations is fixed to 30,000. The fitness function is evolved until it reaches the stabilization position with the best value of 0.0008. Thus, the algorithm parameters are varied according to the evolution of the fitness function that the purpose is to ensure the stability and the control of particles positions and their movement towards the global best position.

The test parameters for the particle swarm optimization are shown in Table.1. The parameters used to optimize the total voltage are presented in Table. 2. The simulation process is carried out on a Pentium 4, 2.5 GHZ 320 MB RAM computer, under windows 7 environment and MATLAB 7.2 software.

TABLE II. Optimized total voltage parameters obtained by particle swarm optimization algorithms.

Parameters	PSO
l [nm]	605
D [nm]	25
F [nN]	80
ρ[cm.Ω]	1
n [ ]	102
a0 [ ]	0.175
a1 [ ]	-0.085
a2 [ ]	0.013
a3 [ ]	-8.61 x 10-4
b0 [ ]	0.714
b1 [ ]	-0.376
b2 [ ]	0.067
b3 [ ]	-0.0040

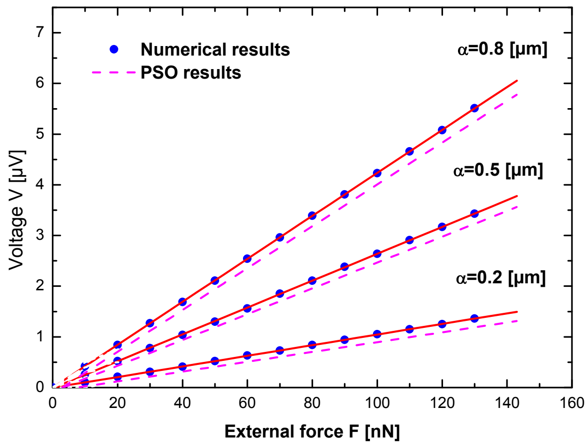

Figure 3. The initial voltage as a function of force with diferrents ratio of length on nanowire diameter.

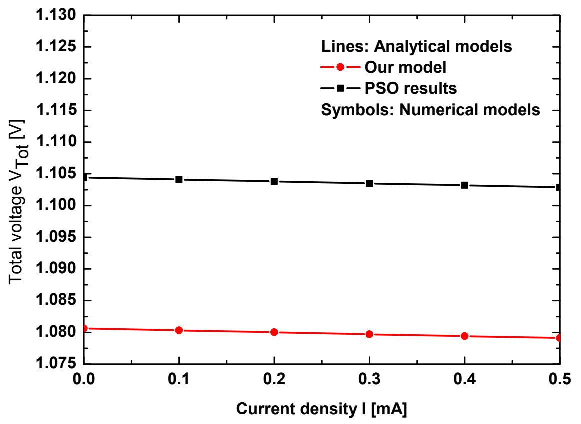

Figure 4. The total voltage generated by the nanogenerator as a function of the current desity.

The initial voltage of the nanowires presents the most critical part of the total voltage. The numerical database has been used to develop the models of initial potential and the total voltage. From Fig. 3 an approximate expression of the initial voltage can be expressed as:

$$V_0 = a(\alpha).F + b(\alpha) \quad (13)$$

where a , b are parameters depending on NWs size and have to be determined by fitting; $\alpha = l/D$. In case of stretch mode the expressions of $a(\alpha)$ and $b(\alpha)$ can be expressed as:

$$a(\alpha) = a_3.\alpha^3 + a_2.\alpha^2 + a_1.\alpha \ + a_0 \quad (14)$$

$$b(\alpha) = b_3.\alpha^3 + b_2.\alpha^2 + b_1.\alpha \ + b_0 \quad (15)$$

where $a_0,\ldots,a_3$ and $b_0,\ldots,b_3$ are the fitting parameters. Substituting Eqs. (6) and (13) into Eq. (5) yields to an analytical voltage model that will be optimized using PSO algorithm. In this context, PSO algorithm is employed with other parameters. For the PSO algorithm the vector $X_j = (F, L, \rho, D, n)$ was optimized, where the fitness value is equal to 1.1002. In this case, the results took about 16.74 min. In order to validate PSO algorithm performances, the starting numerical voltage model was compared to those optimized by PSO procedure. Fig. 4 presents the obtained optimized voltage model as a function of current intensity. The current (I), voltage (V) and power (P) characteristics are compared to those of the conventional model. Table 3. Moreover, the proposed NG device exhibits better performance in comparison to the conventional design for wide range of I, V and P.

TABLE III. COMPARISON BETWEEN THE OPTIMIZED NG AND CONVENTIONAL NG DESIGN PARAMETERS.

Parmeters	Model without optimization	Model with optimization	Coventional one [4]
Voltage [V]	1.08	1.10	0.8
Current [nA]	0.2	0.26	0.1
Power [nW]	0.216	0.286	0.18

For a numerical solution of Eq. (5), the developed structure has been meshed with tetrahedrons shape of 21nm maximum. The considered mesh is fine and not uniform to enable converging on a solution. Fig. 5 shows the obtained electric potential of the NG using finite element simulation in stretch mode respectively.

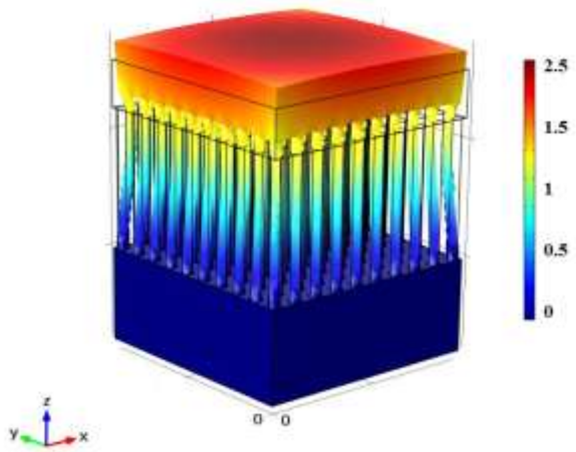

Figure 5. The potential electrique of the nanogenerator..

When applying an axial force on the nanowires, a stress profile is generated along these nanowires. In Fig. 5 it is clear that the electrical potential is distributed along the NWs surfaces, and the behavior of the NG is an image of a single NW behavior. The increase in potential at the top end is due to the effect of local stress created by the axial force applied to this region.

The NG is put in a circuit containing a load and acts as a power source Fig. 2. The voltage generated by the NG device is tested and measured for different lengths of the NWs and different values of the excitation forces. The set of data constitutes the numerical values that are exploited to determine an analytical model.

IV. Conclusion

In this work coupled numerical modeling and heuristic algorithms for NG behavior analysis was presented. Furthermore, a its numerical modeling has been carried out and developed in stretching mode in order to calculate and compare the total voltage generated by the NG. In addition, the applicability of PSO algorithm to study the total voltage generated by the NG has been presented. The PSO algorithm has shown high accuracy to study the total voltage generated by the NG. It is shown that PSO technique can be used in parameters optimization of total voltage generated by the NG. All in all, this study indicates that the developed investigation can be integrated into simulator devices to study the NG-based circuits.

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