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Theoretical study of electro-mechanical energy conversion in ZnO nanowire-based nanogenerator

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Abstract—In the present work, we report the results of theoretical study of electro-mechanical energy conversion using finite element method to model a unit cell of a nanogenerator (NG) with ZnO nanowires (NW). First, we verified the correct coupling of the piezoelectric and semiconducting properties of the ZnO by comparison between analytical and numerical solutions. Then, to know the efficiency of the energy conversion, we compared the electrical energy stored in the unit cell in different cases by modifying some relevant parameters.

I. INTRODUCTION

The harvesting of even small amounts of energy from free micro-sources is a strategic research area for consumer, industrial, military and medical electronics. Indeed, it meets a double objective: making autonomous sensors, which, for various reasons have a complicated energy "recharge" and responding to the issue of sustainable development by reducing the use of batteries and other accumulators. Developing micro- or nano-generators is therefore an important part of the research because they are essential building blocks in the development of autonomous systems (e.g. for transport [1] or space [2]) or communicating systems (e.g. the Internet of Things IoT [3]). In the context of mechanical energy harvesting from movements, different technologies exist. Among them, the direct piezoelectric effect allows a coupling of mechanical and electrical properties. One of the difficulties is to be able to compare the performances of the different systems using an adapted Figure of Merit (FoM) [4]. Since 2006 [5], piezoelectric semiconducting nanowires (e.g. zinc oxide ZnO, gallium nitride GaN...) have appeared as potential candidates for lead-free piezoelectric materials, with enhanced properties compared to their bulk counterparts [6].

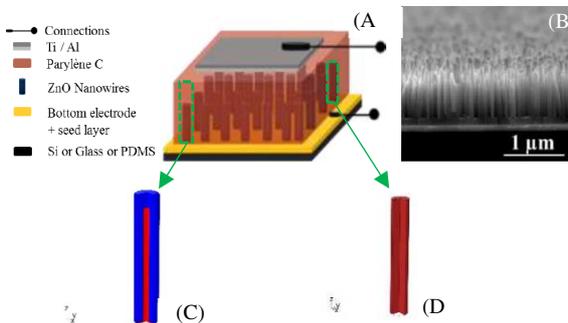


FIGURE 1. (A) DESIGN OF A NANOGENERATOR, (B) SEM IMAGE OF ZnO NW GROWN ON ZnO SEED LAYER (C) UNIT CELL (1) ZnO NW WITH EMBEDDED POLYMER (D) UNIT CELL (2) ZnO NW ONLY

Since then, many experimental or theoretical studies dedicated to ZnO based NG have shown significant improvement of their performances [7]. In the simulation tools, the models must take into account the coupling of two physical phenomena: piezoelectricity and semiconducting properties of this material.

II. MODELLING CONTEXT

A. Unit cells in a zinc oxide nanowires based nanogenerator

At GREMAN laboratory, ZnO NW based NG are designed in a capacitive configuration. They consist in a five-layer device that can be rigid or flexible depending on the type of substrate.

B. Coupling piezoelectric and semiconducting properties

The present study uses the model of the unit cell (2) for a comparison between analytical and numerical results to verify a previous coupling implemented in COMSOL Multiphysics® [8]. In this model, we study the 1D-phenomena along z-axis using the piezoelectric and semiconducting equations to solve Newton's law and Gauss' law in static conditions [9].

The analytical solution for the piezopotential is:

$$V(z) = \frac{d_{33}T}{\epsilon_{33}^T \sqrt{\frac{qn_0\mu_{n,33}}{\epsilon_{33}^T D_{n,33}}} \cosh\left(\sqrt{\frac{qn_0\mu_{n,33}}{\epsilon_{33}^T D_{n,33}}} L\right)} \sinh\left(-\sqrt{\frac{qn_0\mu_{n,33}}{\epsilon_{33}^T D_{n,33}}} z\right) \quad (1)$$

with d_{33} and ϵ_{33}^T the ZnO piezoelectric coefficients, $\mu_{n,33}$ and $D_{n,33}$ the ZnO semiconducting ones, q the elementary charge, $n_0 = 10^{15} \text{ cm}^{-3}$ the n-doping, $2L = 1.2 \mu\text{m}$ the NW length and $T = 0.3272 \text{ MPa}$ the compression stress along z-axis. Regarding the electrical boundary conditions, the unit cell has a floating potential on the top face and an ohmic contact is on the bottom face. FIGURE 2 shows the fit between the analytical and numerical solutions.

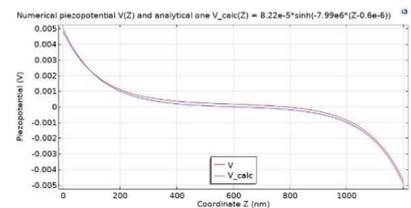


FIGURE 2. COMPARISON BETWEEN THE ANALYTICAL AND NUMERICAL SOLUTIONS OF THE PIEZOPOTENTIAL

C. Energy transfers and conversion

The nanogenerator aims to harvest ambient mechanical energy $\mathcal{E}_{in,mecha}$ and convert it into electrical energy $\mathcal{E}_{out,elec}$. Then its global efficiency E can be defined by:

$$E = \frac{\mathcal{E}_{out,elec}}{\mathcal{E}_{in,mecha}} \quad (2)$$

The full conversion is divided into N steps of energy transfer or conversion, each of them presenting a given efficiency E_i [10]. Then, the global efficiency defined in Eq. (2) is also:

$$E = \prod_{i=1}^N E_i \quad (3)$$

The unit cells (1) and (2) (cf FIGURE 1 (C) and (D)) have the same type of output energy that is the electrical energy stored in the equivalent capacity $\mathcal{E}_{stored,elec}$ given by:

$$\mathcal{E}_{stored,elec} = \frac{1}{2} \iiint_{\text{Unit cell}} \vec{D} \cdot \vec{E} dV \quad (4)$$

where \vec{D} is the displacement field and \vec{E} the electric field. If we consider an open-circuit for the unit cell, we can say that this stored electrical energy is also:

$$\mathcal{E}_{stored,elec} = \frac{1}{2} QV_{oc} \quad (5)$$

where Q is the charge on the top of the cell and V_{oc} the piezopotential in open-circuit configuration (i.e. no load connected to the cell).

III. SIMULATION RESULTS

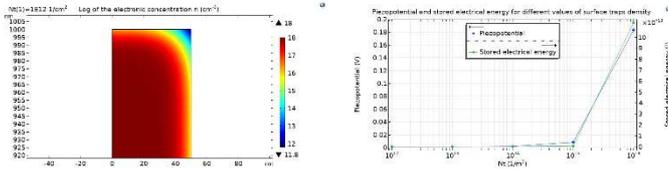


FIGURE 3. (A) IMAGE OF THE TOP OF THE NW WITH DEPLETION ZONE, (B) PIEZOPOTENTIAL AND STORED ELECTRICAL ENERGY FOR DIFFERENT VALUES OF SURFACE TRAPS DENSITY

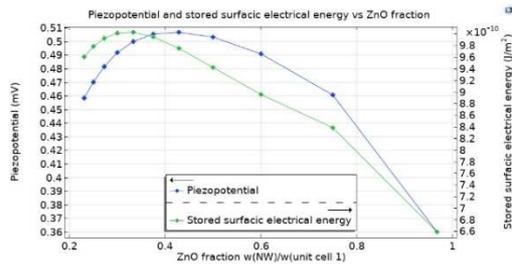


FIGURE 4. PIEZOPOTENTIAL AND STORED ELECTRICAL ENERGY DEPENDING ON THE ZNO FRACTION

A. Surface traps influence

Surface traps can modify the electronic concentration of N-doped NW by creating a depletion zone [11] as in FIGURE 3.(A) for unit cell (2). This effect is strong for a surface traps

density of 10^{12} cm^{-2} in our semiconducting NW as we can see in FIGURE 3.(B).

B. ZnO nanowires density influence

With periodic conditions on the lateral faces of the unit cell (1) (FIGURE 1.(C)), we have studied the influence of the density of the NW by varying the polymer width, while keeping the NW diameter constant. These results confirm that there is an optimal ZnO fraction (FIGURE 4) for the stored electrical energy.

IV. CONCLUSION

The electro-mechanical energy conversion in ZnO NW-based nanogenerator has many influent parameters that can be set or that are inherent of the materials as the screening effect due to the ZnO semiconducting properties. A new step of the model will be to insert some thermal, mechanical and electrical losses in a dynamic study by taking complex materials coefficients (loss angles). Some other additional phenomena as triboelectricity that can appear with PDMS [12] will be studied using surface charge densities.

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