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Stress cycle on a ZnO nanowire-based nanogenerator: a phenomenological study

Emmanuel DUMONS^{1*}, Guylaine POULIN-VITTRANT¹ and Louis Pascal TRAN-HUU-HUE¹

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Abstract—Energy harvesting using nanogenerators is a complex process that starts with the scavenged mechanical energy and ends with the electrical energy given to a load. During this process, many phenomena appear at different steps and in different parts of the device. This work shows with an original point of view that in nanogenerators, energy conversion depends on intrinsic parameters such as zinc oxide doping level or polymer dielectric permittivity. By considering the whole energy conversion chain, this study investigates the important characteristic times adaptation between mechanical excitation and electrical transfer to load.

I. INTRODUCTION

Mechanical energy harvesters are promising devices to make integrated sensors or actuators autonomous by scavenging free energy from the environment [1]. Piezo-nanogenerators use direct piezoelectric effect to harvest an external mechanical energy and convert it into electrical one. For this purpose, ZnO (zinc oxide) nanostructures are used as piezoelectric material and are embedded within a polymer matrix. Many additional phenomena appear during the energy conversion within these nanogenerators: the ZnO semiconducting properties create screening effect due to the free charge carriers and surface effects, the polymer has mechanical and electrical influence [2]...

The aim of this work is to search influent parameters on the energy conversion and transfer to the external load such as mechanical excitation time-dependence, ZnO doping level, polymer dielectric permittivity and external load resistance.

II. DEVICE AND MODEL DESCRIPTION

A. Nanogenerator

To harvest external mechanical energy, the nanogenerators considered here have ZnO piezo-semiconductive vertical nanowires as active elements embedded in a polymer matrix. Including the substrate and the electrodes, these nanogenerators are five-layer devices that electrically work in a capacitive mode due to the polymer layer on the top of the nanowires [3].

B. Unit cell for simulations

To study the different physical phenomena involved in the energy harvesting process, the nanogenerator is studied through a 2D-axisymmetric unit cell composed of a single ZnO nanowire with a polymer layer above. This single cell study allows to predict the full device performance [4]. Due to the unit cell geometry and to the kind of mechanical excitation, we can consider that the piezoelectric material is excited in the 33-mode only. Metallic top and bottom electrodes allow connecting this unit cell to an external circuit. The role of the substrate is not studied in this model. Simulations are performed with *COMSOL Multiphysics*® using our custom-made simulation module coupling piezoelectric and semiconducting properties of ZnO.

The geometric parameters are kept constant in the present study as they were studied previously [5].

C. Stress cycle and boundary conditions

The external mechanical excitation onto this unit cell is a four-step variable pressure applied on top of the unit cell (increasing ramp, constant pressure, decreasing ramp and zero pressure, all of them having the same duration $\tau_{\rm m}$). It creates a stress cycle on the unit cell. The boundary conditions are reported in TABLE 1.

TABLE 1. UNIT CELL BOUNDARY CONDITIONS

	Boundary conditions	
Unit cell boundaries	Mechanical	Electrical
Polymer top surface	Pressure	Circuit terminal (top electrode)
Polymer lateral surface	Free	Zero charge
Polymer/ZnO interface	Continuity	Insulator interface
ZnO lateral surface	Free	Insulation
ZnO bottom surface	Roller	Ohmic contact (bottom electrode)

D. Connection to an external circuit

In the present study, the harvested energy is transferred from the nanogenerator to a resistor R representing the electrical load. The harvested energy is then only dissipated by Joule effect during the discharge of the unit cell. This phenomenon introduces a new time $\tau_{\rm e}$ that corresponds to an electrical characteristic time.

III. RESULTS AND DISCUSSION

A. Electrical energies evolution

Because of the direct piezoelectric effect, a polarization appears within the nanowire and creates an electric field in the unit cell.

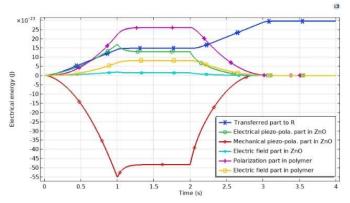


FIGURE 1. ELECTRICAL ENERGIES EVOLUTION

FIGURE 1 presents the evolution of the different electrical energies in the nanowire and in the polymer due to the pressure variation. The graph also includes the amount of energy transferred to the external circuit (dark blue curve).

B. Electrical cycle (E_3, D_3)

To better assess the efficiency of energy transfer to external load, the electrical cycle (E_3,D_3) area in J.m⁻³ represents:

$$\omega_{el} = \oint D_3 \mathbf{d}E_3 \tag{1}$$

the electrical energy density stored in the ZnO nanowire. The local fields are evaluated at the center of the nanowire in order to plot the cycle in FIGURE 1. The electrical cycle presents also four steps corresponding to the mechanical cycle ones.

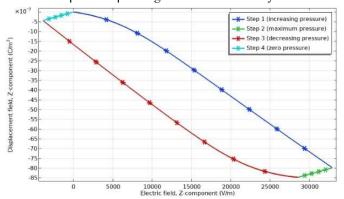


FIGURE 2. ELECTRICAL CYCLE

C. Influence of the ZnO doping level

Due to the semiconductive properties of ZnO, the screening effect of the piezopotential occurs and decreases the harvested energy. The ZnO doping level depends on the nanowires fabrication process [6]. The area of the electrical cycle decreases when the doping level increases.

D. Influence of the polymer dielectric permittivity

The polymer dielectric permittivity is an important parameter due to the capacitive effect introduced by the polymer layer above the ZnO nanowires. The higher the polymer dielectric permittivity, the higher electrical energy transferred to the load as shown in FIGURE 1.

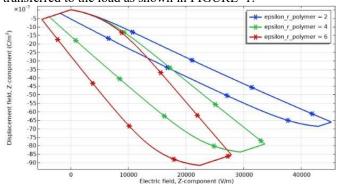


FIGURE 3. ELECTRICAL CYCLE FOR DIFFERENT POLYMER DIELECTRIC PERMITTIVITIES

E. Influence of the external load

By modifying the resistance of the external load, we modify the electrical characteristic time $\tau_{\rm e}$ of the phenomenon. Therefore, we can study the influence of this parameter on the electrical cycle and on the amount of harvested energy. Simulations show that there is a match between the two

characteristic times τ_e and τ_m to maximize the efficiency of the electrical transfer to the external load (FIGURE 1). This result reinforces the interest of using controllable electrical circuits with switching techniques in order to adapt τ_e to τ_m imposed by the external mechanical excitation [7].

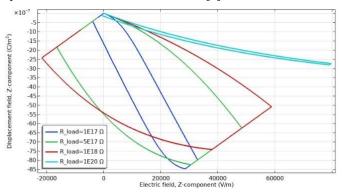


FIGURE 4. ELECTRICAL CYCLE FOR DIFFERENT LOAD RESISTANCES

The cycle with maximum area (red one) indicates the optimal resistance value for a unit cell. By dividing this one by the nanowires number (around one billion) of the prototype described in [3], the full nanogenerator optimal resistance can be estimated [4].

IV. CONCLUSION

Thanks to our simulation tool including coupled physics, this original study of the piezo-semiconducting nanostructure explains the different phenomena involved within the nanogenerator. This provides a better understanding of the full energy harvesting process, combining mechanical energy conversion and electrical charges extraction. This transient analysis opens perspectives to take into account even more realistic mechanical cycles in specific applications. It also shows the influencing parameters that have a real impact on the amount of converted and transferred energy to an external resistor. This time-dependent study will be completed by considering losses in the different materials and ZnO surface traps [5]. Furthermore, other external loads will be used to get closer to a typical circuit following the nanogenerator.

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