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Energy balance numerical study in ZnO nanowire based nanogenerator

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The very important development of connected objects such as multiple sensors to monitor these objects, or actuators to operate them, requires a consequent energy supply. In order to avoid the proliferation of batteries, the idea of making these connected objects autonomous through energy harvesting systems such as piezoelectric nanogenerators is strategic. At GREMAN laboratory, ZnO nanowires based nanogenerators are manufactured on rigid or flexible substrates and consist in a multi-layer device including the ZnO piezo-semiconducting nanowires array embedded in an insulating material. In this energy harvesting application context, a temporal study of the conversion of mechanical energy to electrical one in the device is performed first, then the transfer of this electrical energy to an external circuit is simulated. The different phenomena due to the elastic, piezoelectric and dielectric properties of the device and the different characteristic times (mechanical and electrical ones) can make difficult a fine analysis of the energy conversion. Our numerical model uses the Finite Element Method and is implemented in *COMSOL Multiphysics*®. In a first study, a constant constraint is applied onto a single ZnO monocrystalline piezo-nanowire (without semiconducting properties) in open circuit conditions. Then this nanowire is connected to a resistance to transfer the energy. The evolution of the different energies is explained as on the figure below.

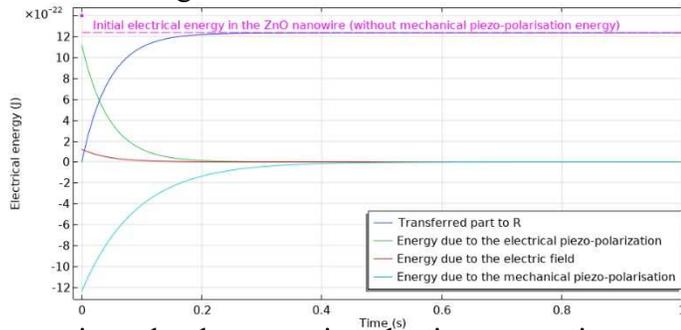


Figure: Evolution of the different parts of electrical energy during the discharge into the resistance R

As ZnO nanowires also have semiconducting properties, we have added, in a second step, an original coupling of piezoelectric and semiconducting properties of ZnO. This numerical coupling has been implemented in the software and has been verified thanks to an analytical model. The second set of studies reproduces the previous simulation parameters but it takes into account the ZnO semiconducting properties. The intrinsic N-doping, with free electrons in the nanowire, increases the electrical conductivity of the material and screens the piezo-potential. One solution consists in adding a layer of dielectric material between the top of the ZnO nanowires and the top electrode that introduces a capacitive coupling. By showing the evolution of the different parts of the energy in the nanowire and in the polymer, the numerical model allows to determine the optimal thickness and permittivity values of the dielectric layer. This will be helpful to identify the best choice of polymer in order to maximize the electromechanical conversion.

Finally, this numerical model is a very powerful tool in which we will take into account the surface traps effect and their consequences on the harvested energy. That will allow us to define, all other characteristics being optimized, the acceptable doping threshold for this application.