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DESIGN AND SIMULATION OF PIEZOELECTRIC TRANSDUCERS WITH OPTIMIZED TOPOLOGY

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Abstract- This paper is devoted to software modeling and simulation of flexible piezoelectric structures, intended for energy harvesting, or sensing applications. The main goal is to enhance their properties in order to efficiently transform mechanical into electric energy and to prove that structured piezoelectric material on flexible substrate can exhibit better conversion ability and sensitivity if suitable geometrical patterns are applied in the films design. This is possible through simulations of different 3D geometric topologies (areas which concentrate mechanical stress in the volume of the structure) with conditions applied from "real work environment" (magnitude, eigenfrequency shapes, frequency range, direction, etc.). With the simulation tools of "COMSOL Multiphysics" different geometries of the piezoelectric structures on flexible substrate of polyethylene terephthalate (PET) were realized and simulated. The chosen piezoelectric material was lead-free potassium niobate ($KNbO_3$). Aluminum electrodes with different geometrical patterns were applied to perform the electrical simulations.

Keywords: Software modeling, Piezoelectric Cantilever, MEMS, Optimized Geometric Topologies, Eigenfrequency, Frequency Range, Piezoelectric Potential, Electrical Simulations.

1. INTRODUCTION

Nowadays, the energy consumption has become higher every year. For this reason, the design rules for the new electronic devices are related to efficiency, low power consumption and reliable power supply. There are some portable devices that require autonomous power supply [1]. The independent sources of energy for microelectronic devices expend exponentially application field and narrows the service maintenance on them. On the first place for independent green energy devices are solar cells followed tightly by piezoelectric "harvesters" [2].

These "harvesters" can produce low electric power when mechanical force is applied due to the piezoelectric effect [3]. Such kinds of devices have widespread applications in micro and nanoelectrical mechanical systems (MEMS and NEMS) [4]. In addition, a lot of sensors, such as pressure and force meters, accelerometers, gyroscopes also work by using the same principle [5].

In both cases (sensing and harvesting) the low frequency processes are of interest due to the nature of the mechanical stimulus. The main disadvantage of piezoelectric microgenerators and microsensors (in general the transducers) is that their conversion ratio (applied load to produced voltage) is too low, because of their small size and low volume (thin film devices).

There are many research papers investigating this issue to obtain better performance [6-9]. One of the approaches to achieve this goal is through optimization of the device geometry. Inner volume and structure of devices are improved in order to obtain areas with higher inner stress. This is possible with using virtual CAD modeling [10]. In order to achieve proper simulation" COMSOL Multiphysics" was chosen. This software product has capabilities to perform and give results on defined tasks [11]. Advantage of the software is that object geometry is build and simulate in low range metric scale (microns and nanometers).

Cantilever type of piezoelectric transducers is widely popular and object of different simulation and modeling investigation (electric, geometric, material types etc.), but the main goal is increasing output parameters of the device [12]. By the author's knowledge, there is not yet reported study exploring the effect of the stress concentrators size and distribution in microscale level on the electrical performance of flexible piezoelectric transducers which are not cantilevers or membranes shaped.

According to the literature review, the application of the thin nanosized film of $KNbO_3$ under the concentrators is also first-time study in COMSOL Multiphysics for such kind of patterned devices. The main goal of this modeling is to determine the optimal Eigen frequency in the range between 40 Hz and 60 Hz, and the optimal electric potential spread in flexible substrate-based structures, fabricated by the same materials and dimensions, but having different geometrical patterns of the top electrode. Simulation of transducers with $KNbO_3$ functional nanocoatings is conducted for determinate optimal pattern for piezoelectric structure. Their Eigen frequencies and modal shapes in predefined range and optimal distribution of piezoelectric potential in the volume of the structure will be investigated.

2. SIMULATIONS AND CONDITIONS

The transducer structure on PET substrate consists of two aluminum electrode layers and one layer of piezoelectric material potassium niobate "sandwiched" in between. The substrate thickness was 125µm and the surface area was 3.15cm^2. Aluminum electrode with thickness of 200 nm with the same area like the substrate was added. On the electrode piezoelectric layer of $KNbO_3$ was grown with a thickness of 570 nm and an area of 2.4 cm^2. In order to complete the sandwich structure, it was formed a top aluminum electrode with a thickness of 200 nm and an area of 2.25 cm^2. All layer's thicknesses were related to different technological processes and modes. They were defined as optimal in our previous research [13]. The layers sequence is show in Figure 1. It was used a simulation model called "cantilever" with boundary conditions "fixed constrain" in order to simulate the composed structure (Figure 2).

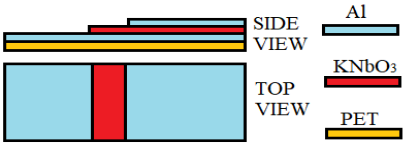

Figure 1. Schematic drawing of the "sandwich" structure and description of the materials involved

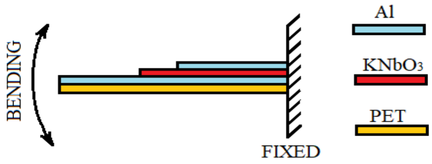

Figure 2. Type of fixation "cantilever "model used for the simulated structures

For the simulation and modeling of the devices' electrical properties variations COMSOL Multiphysics software was used. The analysis implemented finite element model (FEM) on fixed constant "cantilever" geometry. FEM analyze is widely used for simulating physic effects in microelectronic structures MEMS and NEMS [11]. This simulation technique is used in other CAD product like "SolidWorks" and "Ansys". For microelectronic structure in nanorange scale COMSOL Multiphysics have advantages. The software is capable to simulate multiphysical effects in structures within nanoscale range. Some disadvantages like higher calculating resources and longer computing time are needed.

Other product that execute FEM simulation does not need such high resources but in nanoscale range they are unable to perform simulations. An information about the eigenfrequencies and piezoelectric potential were extracted in this way to obtain a suitable electrode geometry with an optimal electrical (power) performance in the range 40Hz - 60Hz. Some physical parameters of the involved materials, such as Young modulus and densities of aluminum, were taken from software library and others form the literature [14] They were summarized in Table 1.

3. RESULTS AND DISCUSSION

The simulation launched with creating the device initial geometry at defined parameters as is shown in Figure 3. All dimensions must correspond to their pre-defined values. This is crucial in order to obtain accurate results. Ordering of the materials used for the simulation is shown in Figure 4. They have typical properties values and units as described in Table 1. Those values determine all possible modes in all directions in 3D study and distribution of electric potential in the volume of investigated structures as well.

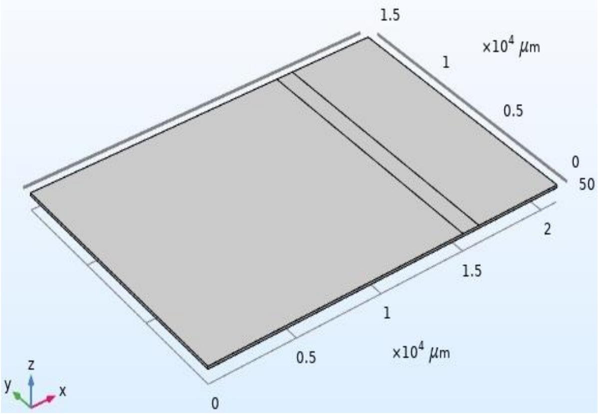

Figure 3. 3D view of the device geometry with defined parameters in COMSOL Multiphysics

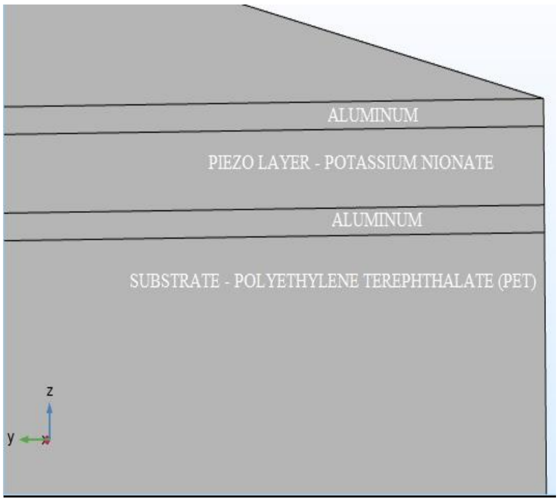

Figure 4. Layers, materials and ordering of the structure

Table 1. Geometric and material parameters used for the simulation

Parameters	Description	Values	Units
L	Beam length	21	mm
b	Beam width	15	mm
h_p	Piezoelectric layer thickness	570	nm
h_s	Substrate layer thickness	125	µm
h_e	Electrode layer thickness	200	nm
Ys	Young's modulus of substrate material	2.95	GPa
Yp	Young's modulus of piezoelectric material	90	GPa
ρ_s	Mass density of substrate material	1380	kg/m^3
ρ_p	Mass density of pizoelectric material	4624	kg/m^3

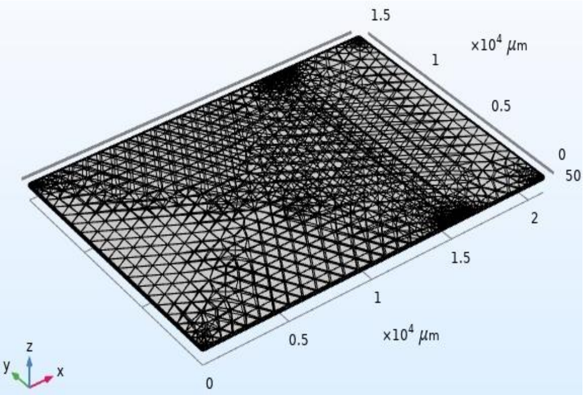

Figure 5. "Meshing" the structure to implement the simulation

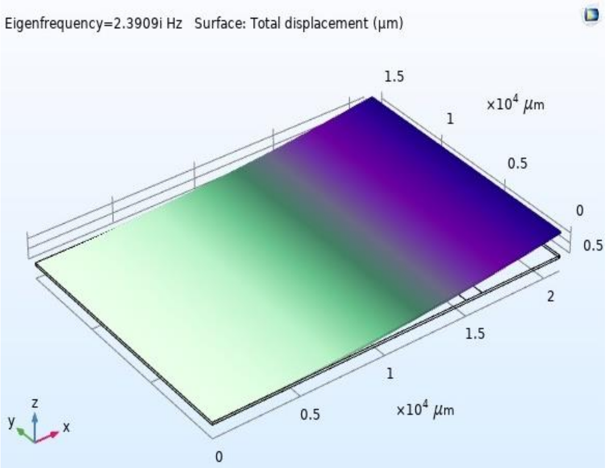

Figure 6. Simulation results for eigenfrequency of unoptimized piezoelectric device

The first (2.4 Hz) and the second (283 Hz) Eigenfrequencies showed that the electric potential with initially defined geometrical parameters but without specific patterns is out of the predefined functional range from 40 Hz up to 60 Hz (Figures 7 and 8).

In order to obtain better performance, the top electrode was formed with comb-shaped geometry. This is conventional structure of electrodes for microelectronic and microelectromechanical devices [15].

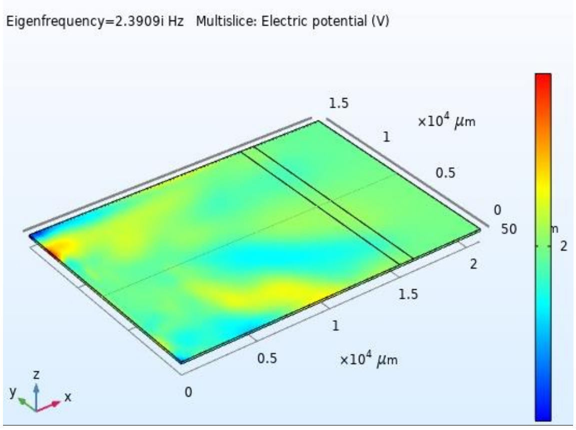

Figure 7. Electric potential on non-optimised geometry at the first eigenfrequency of 2.4 Hz

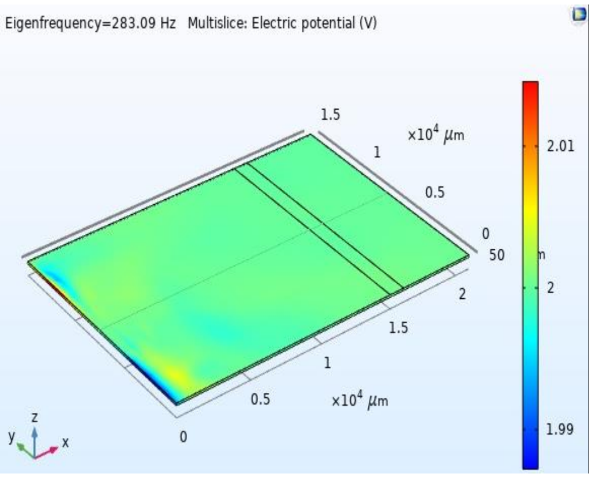

Figure 8. Electric potential on unoptimised geometry at Second eigenfrequency of 283 Hz

The simulation results showed that the first Eigen frequency was 3.52 Hz which is not in the predefined range. Distribution off inner stress areas is uneven and concentrated around angles of the structure and electric potential above 2V can be found around angels and layers boundaries. (Figure 9). This result indicated that a need of a geometry pattern change appeared. To optimize simulation, it was chosen pattern with circular stress concentrators due to their abilities to concentrate mechanical stress in the volume of the structures [16].

In this type of geometric patterns, inner stresses are evenly distributed for that reason longer life of the device is possible. If structure with angular shape is used to concentrate mechanical stress (Figure 9), there is possibility of cracks on angles during the bending cycles.

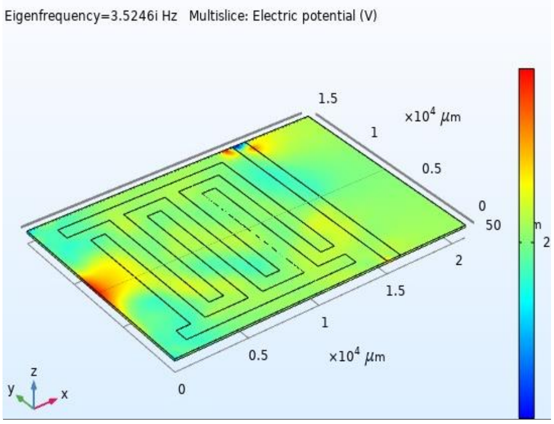

Figure 9. Comb-shaped top electrode-electric potential distribution and eigenfrequency of 3.5 Hz

To determinate optimal diameter of the concentrators the first circular topology consists "small" (1300 μm) and "big" (2300 μm) concentrator diameters. It is observed that higher inner stress and electric potential charges are observed around bigger diameter concentrators and eigenfrequency of 39 Hz which is in lower zone of predefined frequency rage (Figure 10).

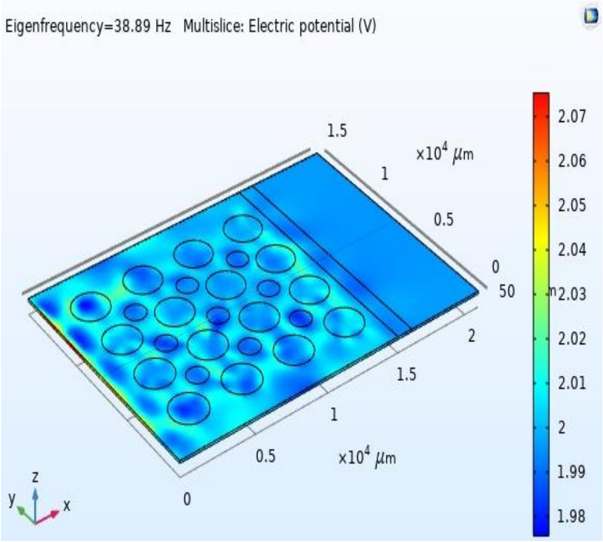

Figure 10. Combined size diameters concentrators on the top electrode layer - electric potential and eigenfrequency of 39 Hz

To achieve an optimal eigenfrequency of 50 Hz (in the middle of the predefined working range) structure with bigger diameter (2300 µm) of concentrators and previous pattern configurations were simulated (Figure 11). Electrical charge and inner stress are evenly distributed, but electric potential is above 2V in a few areas (around 5% off inner volume).

The eigenfrequency of 43.5 Hz is still out of predefined optimal frequency rage. The best parameters were achieved for a structure with nine stress concentrators having diameter of 2.6 mm each. The result represented even inner stress distribution with the highest electric potential and eigenfrequency of 48 Hz (Figure 12). In this geometric configuration simulated structure show highest electric potential of 2.07 V related to around 50% off inner-structural volume.

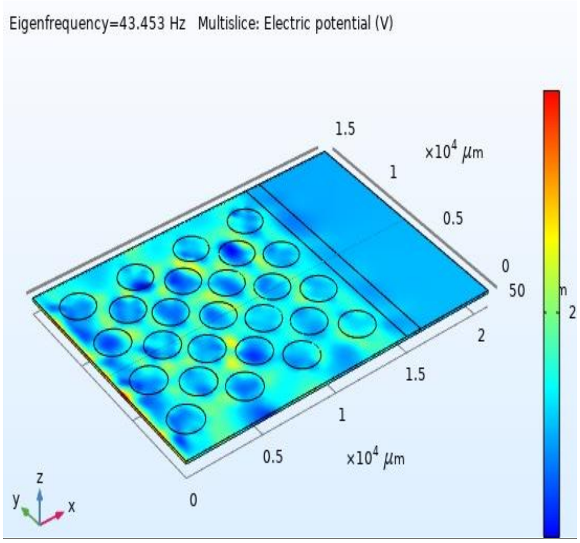

Figure 11. Optimized with "x pattern" circular concentrators with the same size diameters and eigenfrequency of 43.5 Hz

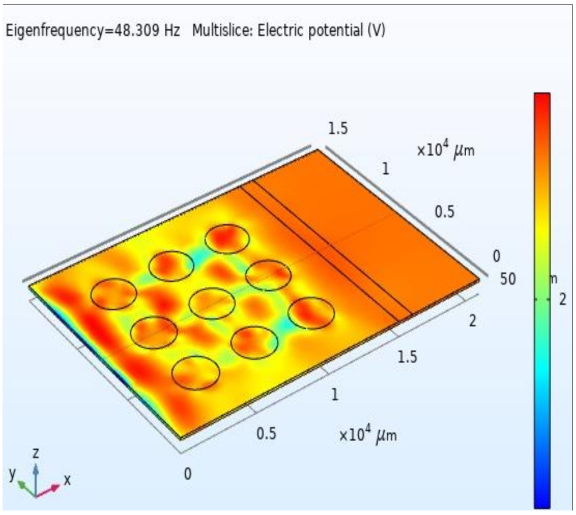

Figure 12. Optimal structure with nine circular concentrators with same diameters (optimal inner stress distribution and eigenfrequency of 48.3 Hz)

4. CONCLUSIONS

Widely spread piezoelectric cantilever flexible structures, with optimized topology, frequency range and electric potential was designed and simulated. The transducer converts maximum energy when the source frequency matches the natural frequency. That's why variety of geometries were studied and the most suitable one was proposed for further fabrication of the device covering the middle range of the predefined frequency range. The geometry of the structure and the FEM analysis were performed in the simulation system of "COMSOL Multiphysics".

The different geometries of the device affect their dynamic and electrical parameters. Simulated results shoes that certain circular geometrical structuring of upper electrode, combined with matching the natural frequency with source frequency in predefined range can optimize electric potential in inner-structural volume of the device. It was achieved highest electric potential of 2.07V distributed in around 50% off inner-structural volume with eigenfrequency of 48.3 Hz. The optimal value of the electric potential (2.07 V) is found for maximum power generation.

All simulated structures with optimized geometrical topology have the same volume of structuring materials except the top electrode. By using simulation approaches for MEMS and NEMS elements, it is determined the optimal topology for the structures. In this way, the fabrication cost and time spent for trial-error iterations during the manufacturing of flexible thin film piezoelectric transducers are significantly reduced. Future work will present further optimization of the simulated structures. This might be possible with structuring of the piezoelectric material in defined pattern combined with patterned electrodes. This could be simulated in "COMSOL Multiphysics" as well to reach even higher inner stresses and piezoelectric potential. In addition, nanosized diameters of concentrators is also of interest for studying.

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BIOGRAPHY

Tsvetozar D. Tsanev was born in Stara Zagora, Bulgaria, 1989. He received his B.Sc. in mechanical engineering in 2013 and M.Sc. degree in electronics in 2016, both from Technical University of Sofia, Sofia, Bulgaria. Currently, he is a Ph.D. student at Department of Microelectronics, at the same university. His current research interests include microelectronic technologies, MEMS, piezoelectric energy harvesting, nanostructuring, flexible electronics, thin films.