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SECTION 2. Applied mathematics. Mathematical modeling.

COMPARISON OF QUARTZ AND LEAD ZIRCONATE TITANATE EFFECT IN THE MANUFACTURE OF ACOUSTIC MICRO PROBE TO STIMULATE THE NEURAL TISSUE AND CREATE AN ACTION POTENTIAL AND ITS SIMULATION BY COMSOL MULTIPHYSICS SOFTWARE

Abstract*: In this paper, design and simulation of acoustic micro probe made of piezoelectric materials such as Lead Zirconate Titanate (pzt) and Quartz to stimulate nerve tissue and produce the wave of action potential in order to transmit the nerve messages inside of axoplasm of an axon have been explored. The simulation has been performed. by using the Comsol Multiphysics 3.5a software. In this simulation, we have designed a piezoelectric blade that part of it is placed inside of ionic enviroment that made of saline matter. By applying the voltage on outer side of blade, due to piezoelectric materials propertis, the blade vibrated and lead to displacement of sodium and chloride ions. This movement of ions creates a current within the ionic enviroment. Then, by applying the obtained current as input to fitzhugh nagumo model,we succed to produce the wave of action potential inside of axoplasm of an axon. The remarkable thing is that, in simulation of piezoelectric blade we used Lead Zirconate Titanate and Quartz and after completing the simulation process, Despite the large difference in the density of the material, due to the proximity of the voltage value at the different time of propagation of the action potential, less dense materials such as quartz can be used in acoustic micro probe designation in order to nerve stimulation.*

Key words*: Piezoelectric, Lead Zirconate Titanate, Quartz, Fitzhugh Nagumo, Action Potential, Axon.*

Language*: English*

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Introduction

The nerve cell, or neuron, is the key player in the activity of the nervous system. It conveys information both electrically and chemically. Within the neuron itself, information is passed along through the movement of an electrical charge (i.e., impulse). The neuron has three main components: (1) the dendrites, thin fibers that extend from the cell in branched tendrils to receive information from other neurons; (2) the cell body, which carries out most of the neuron's basic cellular functioning; and (3) the axon, a long, thin fiber that carries nerve impulses to other neurons[1].

When the membranes of neurons is stimulated,a bioelectric change that occurs in the nerve membrane and propagate from the stimulation site to other parts of the nervous fiber. This phenomenon is called action potential. In other word, the action potential occurs on a excitable membranes of nerve cells, over the length of the axon and has the task of messaging[2]. Each action potential start with suddenly change in negative natural potential (rest mode) to positive potential of memrance and come back with the same speed in the negative mode and ends[3]. To convey a message of nerve, action potential travels along the nerve fibers to reach the nerve endings.

Lead Zirconate Titanat

Lead zirconate titanate (in short PZT) is one of the most frequently studied ferroelectric materials, due to its extremely wide field of application as a pyroelectric material. Lead zirconate titanate Pb($\mathbf{Zr}_{1-x}$Tix)O3 is a solid solution of ferroelectric

PbTiO3 (Tc=490C) and antiferroelectric PbZrO3 (Tc=230C). PZT properties depend on the ratio of Zr/Ti. In the room temperature Tr = 20C PZT is a ferroelectric, so it possesses also piezo and pyroelectric properties for: 0.042 < x < 0.380 (rhombohedral R3c), 0.380 < x < 0.470 (rhombohedral R3m) as well as 0.480 < x <1.000 (tetragonal P4mm). Solid solutions from the area of 0.47< x < 0.48 in T > 227 C constitute a mixture of tetragonal and rhombohedral phase, in Tr = 20 C they indicate monoclinic system symmetry (it is so called morphotropic phase boundary region). Physical properties of the PZT ceramics depend on technology, especially on temperature and time of densification because during the densification process evaporation of lead can be observed, which causes disturbance in the initial chemical composition. In practice, PZT is rarely used in a pure chemical form. The dielectric, piezoelectric and pyroelectric properties of PZT can be modified by adding dopants [4].

Appropriate choice of a type and a quantity of dopant ions is important. There are reports about obtaining Mn-doped Pb(Zr0:3Ti0:7)O3 ceramics (by conventional ceramic method) [5-7] and thin films [8,9] for pyroelectric applications. Doping manganese into PZT led to a significant increase of the pyroelectric effect and decrease of the dielectric permittivity and dielectric losses coefficient tg[10]. In this work powders preparation of manganese-doped lead zirconate titanate with composition of Pb (Zr0:3Ti0:7) 0:97 Mn0:03O3 (PMZT) is presented. The powders were obtained by sol gel method. The obtained powders were then used for preparing ceramic-polymer composites for pyroelectric applications. Ceramic polymer composites have lots of advantages in comparison with monolithic ceramics and thin films. They can be prepared at low cost in any sizes and shapes required for specific uses [11].

Quartz

The technical formula is SiO2 and it is composed of two elements, silicon and oxygen. In its amorphous form SiO2 is the major constituent in many rocks and sand. The crystalline form of SiO2 or quartz is relatively abundant in nature, but in the highly pure form required for the manufacture of quartz crystal units, the supply tends to be small. The limited supply and the high cost of natural quartz have resulted in the development of a synthetic quartz manufacturing industry. Synthetic quartz crystals are produced in vertical autoclaves. The autoclave works on the principle of hydrothermal gradients with temperatures in excess of 400 °C and pressures exceeding 1,000 atmospheres. Seed quartz crystals are placed in the upper chamber of the autoclave with natural quartz (lascas) being placed in the lower chamber. An alkaline solution is then introduced which when heated increases the pressure within the chamber. The autoclave heaters produce a lower temperature at the top chamber in comparison to the bottom. This temperature gradient produces convection of the alkaline solution which dissolves the natural quartz at the bottom of the chamber and deposits it on the seed crystals at the top. Alpha crystals produced by this method can have masses of several hundred grams and can be grown in a few weeks. If the temperature reaches 573 °C a phase transition takes place which changes the quartz from an alpha to a beta (loss of piezoelectric property). Quartz crystals are an indispensable component of modern electronic technology. They are used to generate frequencies to control and manage virtually all communication systems. They provide the isochronous element in most clocks, watches, computers and microprocessors. The quartz crystal is the product of the phenomenon of piezo-electricity discovered by the Curie brothers in France in 1880[11].

Fitzhugh Nagumo Model

The Fitzhugh-nagumo equations is a simplified form of the Hodgkin-Huxley model for electrical activity in a neuron. in this model a neuron can be stimulated with an input such as an electric current. The state of this excitation is described by variable $\boldsymbol{u_1}$ which represent the voltage (excitation) in the neuron as a function of time. when a neuron is excited, physiological processes in the cell will cause the neuron to recover from the excitation. The variable $\boldsymbol{u_2}$ in the model equation represents this recovery [12],[13]. The equations are given by :

$$\frac{\partial_{u_1}}{\partial_t} = \Delta \boldsymbol{u} + (\boldsymbol{\alpha} - \boldsymbol{u_1})(\boldsymbol{u_1} - \mathbf{1})\boldsymbol{u_1} + (-\boldsymbol{u_2}) + \boldsymbol{I} \quad (1)$$

$$\frac{\partial_{u_2}}{\partial_t} = \boldsymbol{\varepsilon}(\boldsymbol{\beta u_1} - \boldsymbol{\gamma u_2} - \boldsymbol{\delta}) \quad (2)$$

$\boldsymbol{\alpha}$ is the excitation threshold and $\boldsymbol{\varepsilon}$ is the excitability. $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ are parameters effecting the resting state and dynamics of the system [14].

Simulation

One of the most important software in simulation of finite element method (FEM) and analysis is comsol multyphysics. The distinguishing feature of this software is accuracy and speed of analysis. In this simulation, we have designed a piezoelectric blade made of lead zirconate titanate at first section and quartz in the second section, that part of it is placed within ionic enviroment that made of saline matter. By applying the external voltage on outer side of blade, a current within the ionic enviroment created. Then, by applying this current as input to fitzhugh nagumo model, the wave of action potential inside of axoplasm of an axon produced and propagated over the length of axon. The remarkable thing is that, in order to avoid numerical limits and obtain the more accurate results, the size of piezoelectric blade, axon and ionic enviroment larger than their actual size is considered.

The simulation steps is as follow:

A) Selection of the dimension and type of modules

B) design of model Geometry

C) Determine the Subdomain Settings and boundary conditions

D) Select the materials and its characteristics

E) Mesh Generation

F) Choose the type of analysis

The following we will explain the steps .

A) Selection of the dimension and type of modules

In this simulation, we have used the three-dimensional structure and in order to simulation of piezoelectric blade, ionic environment and axon respectively, piezo solid, electrostatics and PDE modules have been used.

B) design of model Geometry

In simulation of finite element method, to reduce the time needed for model analysis, we use the appropriate geometric approximation to the size limition of the model.

The piezo electric blade modeled as a solid block with size of 15 ×15 ×140 $\boldsymbol{m^3}$ (l ×w ×h), As mentioned in previouse sections, a part of piezoelectric blade is placed in ionic environment that is modeled by solid block with size of 5 ×1 ×40 $\boldsymbol{m^3}$. Also the axons geometry is a hollow cylinder with length of 125 m and radius of 5 cm.

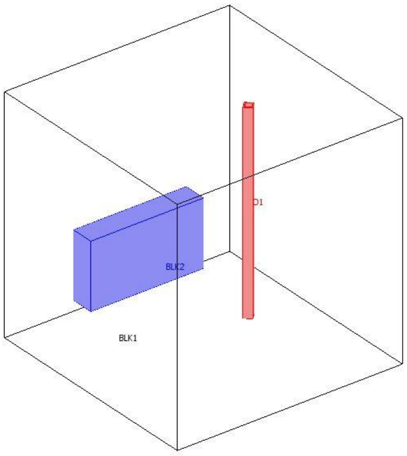


Figure 1 - Geometrical model for simulation.

C) Determine the Subdomain Settings and boundary conditions

C-1) *Subdomain Settings*

In this section of simulation, due to use Lead Zirconate Titanium and Quartz, comsol default setting was used for these materials. So that the density of these matters , respectively are equal to 7600 and 2651[kg/m^3].

The equation that used for ionic enviroment in the electrostatic module , is as following.

$$-\nabla.\,\varepsilon_0\varepsilon_r\nabla V = \rho \qquad (3)$$

Where V is electric potential, ε_r is the relative permittivity, ε_0 is the permittivity of vacuum and ρ is the charge density. Also saline relative permittivity is equal to 80.

In PDE module, the axon subdomain described by two dependant variables , $\boldsymbol{u_1}$ and $\boldsymbol{u_2}$. The equation that solved by PDE mode is as following.

$$e_a\frac{\partial^2 u}{\partial t^2} + d_a\frac{\partial u}{\partial t} + \nabla\Gamma = F \qquad (4)$$

where $\boldsymbol{e_a}$ is mass coefficient, $\boldsymbol{d_a}$ is damping coefficient, $\boldsymbol{\Gamma}$ is numerical flux and F is source term . in order to create the main equations ie (1) and (2) equations, we need to following parameters.

$\boldsymbol{e_a} = 0$, $\boldsymbol{d_a} = 1$, $\boldsymbol{F} = 0$.

The numerical flux $\boldsymbol{\Gamma}$ for equation (1) and (2) is set to:

$$\Gamma = \Delta u + (\alpha - u_1)(u_1 - 1)u_1 + (-u_2) + I \qquad (5)$$

$$\boldsymbol{\Gamma = \varepsilon(\beta u_1 - \gamma u_2 - \delta).} \tag{6}$$

Boundary conditions for the axons as well as the following :

$$\boldsymbol{u_1(t_0) = V_0.\left((x+d) > 0\right).(z+d > 0)} \tag{7}$$

$$\boldsymbol{u_2(t_0) = nu_0.\left((-x+d) > 0\right).(z+d > 0)} \tag{8}$$

C-2) Boundary Conditions

After determining the border areas of piezoelectric blade and applying voltage to the outer area, its time to determin the boundary areas within ionic enviroment and axon. Electric potential distribution in the ionic environment is done by using electrostatic module and Maxwell's equations.

Nonlinear differential equations or Fitzhugh-nagumo as axons describe the cell membrane behavior with respect to the input that we applied to them. All of the axon boundaries in the PDE mode are taken as Neumann boundary condition and the equation that used in boundary mode is as following:

$$\boldsymbol{-n.\Gamma = G\,.} \tag{9}$$

Where $\boldsymbol{\Gamma}$ is numerical flux and G is source term. $\boldsymbol{\Gamma}$ from Equation (5) is obtained and G = 0. all boundaries of ionic environment are at ground potential (V = 0),also all boundaries of the axon are selected as electrical potential with the coupling variable $\boldsymbol{u_1}$=$\boldsymbol{V_0}$[10].

E) Mesh Generation

In this section, we have used the triangular elements in mesh generation process. The reason of using the triangular elements is rising the speed of solving the problem. Also have been tried to use smaller elements in sensitive areas such as axons and piezoelectric blade common border. 19,837 and 19619 is the number of elements used in mesh generation of lead zirconate titanat and quartz.

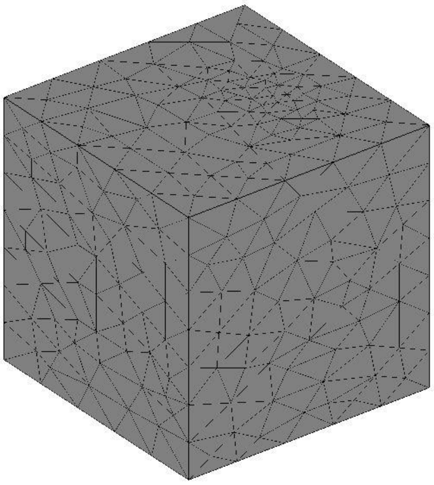


Figure 2 - The meshed model.

POST PROCESSING

After running the simulation, the results obtained and in the first part of the simulation results, we see the action potential propagation inside of axoplasm of an axon due to effection of Lead Zirconate Titanate micro probe on ionic enviroment and in the second part of simulation results, action potential propagation due to effection of quartz micro probe are visible.

A) Lead Zirconate Titanate micro probe results:

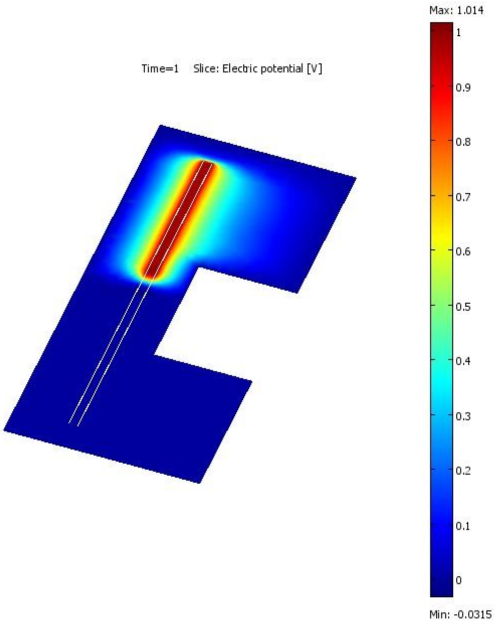


Figure 3 - Action potential propagation inside of axon at 1s.

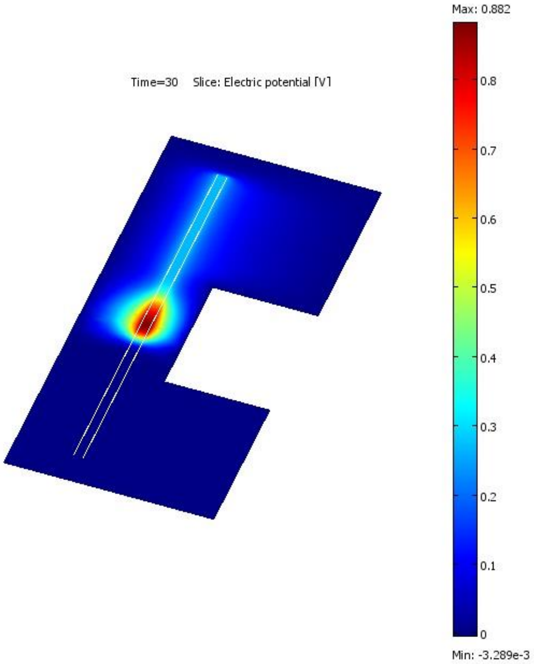


Figure 4 - Action potential propagation inside of axon at 30s.

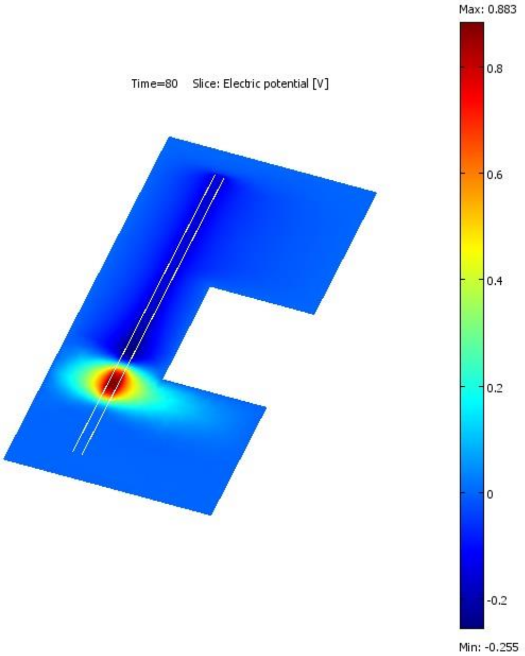


Figure 5 - Action potential propagation inside of axon at 80s.

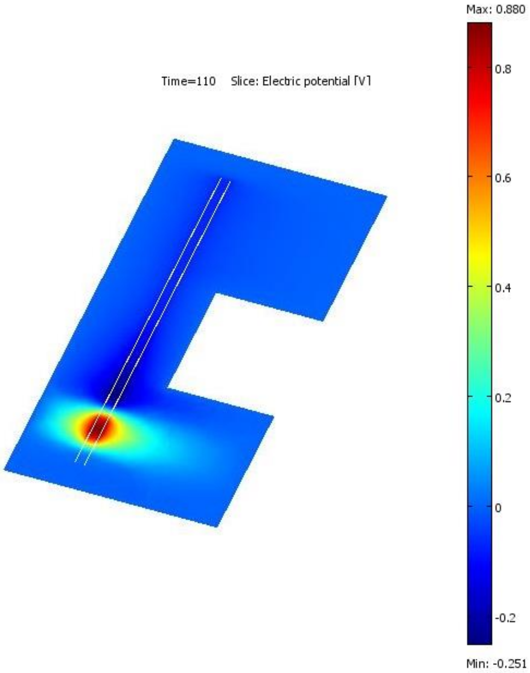


Figure 6 - Action potential propagation inside of axon at 110s.

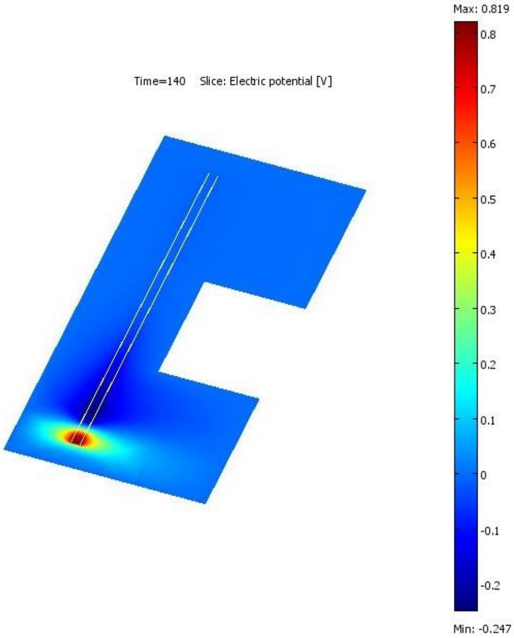
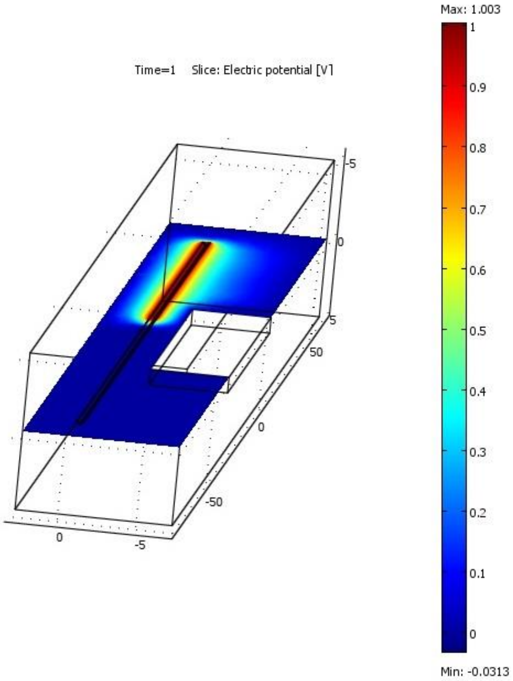


Figure 7 - Action potential propagation inside of axon at 140s.

B) Quartz micro probe results:



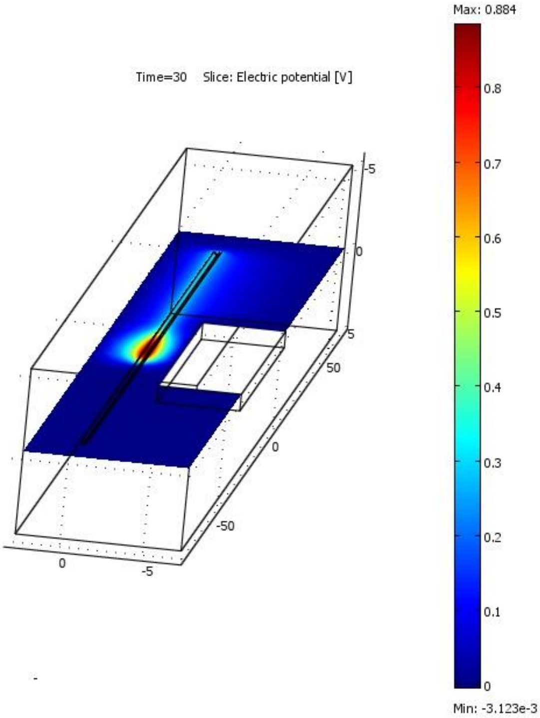


Figure 8 - Action potential propagation inside of axon at 1s.

Figure 9 - Action potential propagation inside of axon at 30s.

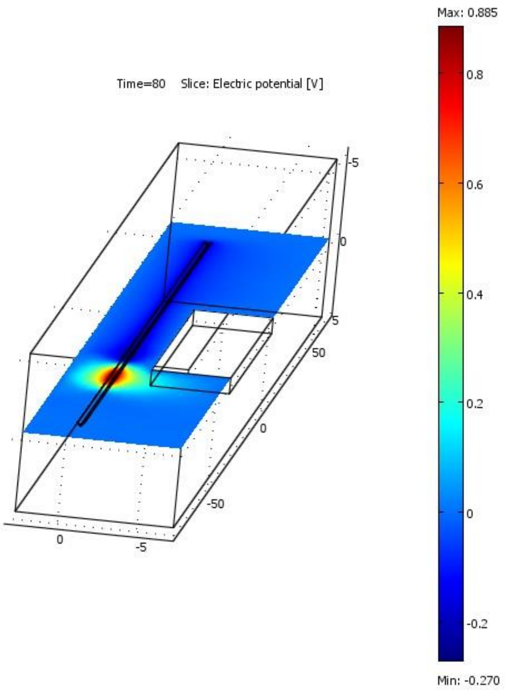


Figure 10 - Action potential propagation inside of axon at 80s.

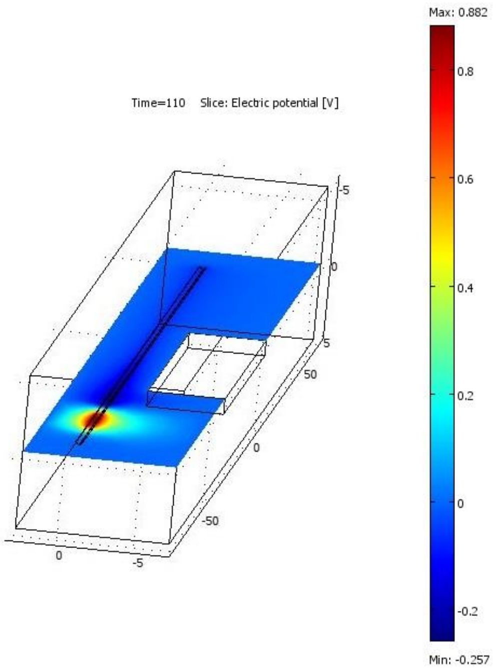


Figure 11 - Action potential propagation inside of axon at 110s.

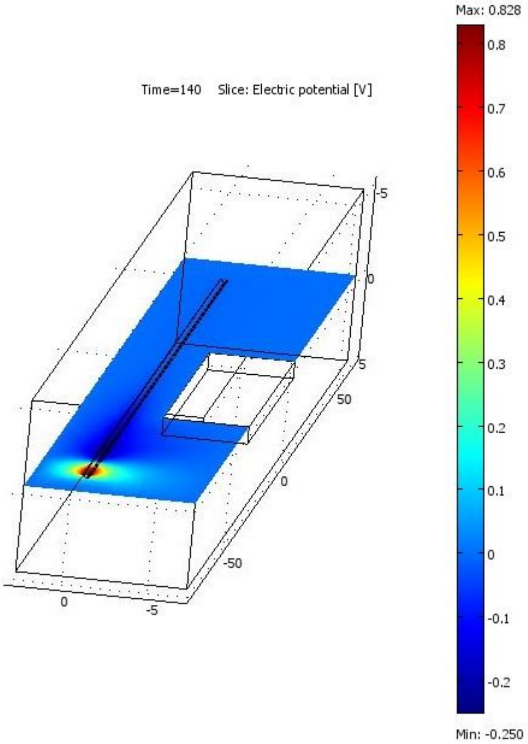


Figure 12 - Action potential propagation inside of axon at 140s.

CONCLUSION

In this paper, we design a piezoelectric blade made of Lead Zirconate Titanate and Quartz. Part of this blade is placed in ionic environment. Since the ionic environment should be similar to the human body and the space around nerve cells so it is made of saline matter. By applying the voltage source to outer side of blade, the blade start to vibrate and this lead to displacement of the sodium and chloride ions, when these ions move inside of ionic environment, a current created. By applying this current as input to Fitzhugh nagumo model, the wave of action potential generated and at different times propagated inside of axon and transmite the neural messages over the length of axon. In this simulation, by comparing the obtained results of Lead Zirconate Titanate and Quartz, It can be concluded that despite the proximity of the action potential wave voltage values, less dense materials such as quartz can be used in acoustic micro probe designation in order to nerve stimulation.

APPENDIX

Table 1

Constants for Fitzhugh Nagumo equations that used in the simulation[10].

Name	Value	Describtion
α	0.1	Excitation threshold [V]
β	0.75	System Parameter
γ	1	System Parameter
δ	0	System Parameter
ε	0.01	Excitability
d	1	Off-axis shift distance [m]
V_0	1	Electric potential
nu_0	0.025	Relaxtion value

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