Design and Simulation of PDMS Based Dry Electrode with impurities using Comsol Multiphysics

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Abstract: *Bio-potentials refer to the voltage produced by a tissue of the body, particular ly muscle tissue during a contraction, these signals are used to analyse various ailments in the medical field like ECG, EEG, and EOG etc. For a single EEG test at least 20 electrodes are required and costs range between 100$ to 500$, hence there is a need to cut down on costs per electrode to bring down the cost of the test as a whole. The conventional electrodes that are used for the measurement of the bio-signals are those of Ag/AgCl wet electrodes, this type of electrodes present challenges such as non-flexibility, irritation to skin and deteriorating signal quality over a longer period of usage, to overcome these shortcomings of the conventional electrodes,*

This paper presents the procedure for simulating the dry electrode that can be used for measuring Bio-medical potentials using Poly Dimethyl Siloxane (PDMS) based electrodes which perform at similar levels as that of the conventional electrodes.

Keywords: Biopotential, Comsol, simulation, flexible dry electrodes, PDMS and MEMS.

1. Introduction

Bio electrodes are extensively used to detect electric signals arising inside the body due to the electro-chemical activity of a certain class of cells, known as excitable cells. Bioelectric phenomena, such as Electro Cardiograph (ECG), Electro Encephalography (EEG) and Electro Occulography (EOG), can be recorded from the surface of the body [1, 2, 3, 4, 5]. These bio-potentials are recorded using bio-electrodes that convert the ionic currents from the body to electric currents or potentials. For a single EEG test at least 20 electrodes are required and costs range between 100$ to 500$. Hence there is a need to cut down the costs per electrode to bring down the cost of the test as a whole. There is a wide variety with different types and shapes of metal electrodes, such as plate and cup electrodes, suction electrodes and floating electrodes [3]. Most widely used metal electrode type is the Ag/AgCl electrode.

One major challenge in recording bio potentials is the electrically insulating outer layer of the skin, i.e. stratum corneum[6]. To overcome this, a conductive gel is used which also results in non-linearity because of varying impedance levels as gel dries up, thus leading to variation of signal quality over long monitoring intervals. The other methods used to obtain the bio potentials include skin abrasion, grooving the skin to insert the electrodes etc, in the conventionally utilized metal electrodes which may lead to skin infections and other complications. The other major disadvantage of the most widely used solid electrodes (e.g. metal plate or cup) is their inability to conform to the irregularly shaped skin surface that additionally can change its local curvature during movement. Thus materials that are flexible need to be used to develop the electrodes.

To overcome above mentioned difficulties there is a need to develop dry and flexible electrodes [12], which performs at similar levels (performance, durability, flexibility, mechanical stability etc.) as the conventionally used metal electrodes. PVDF and PDMS are dry electrodes that can be used instead of the conventional wet electrodes. PVDF is not as flexible making it difficult to sense the bio medical signals. The PDMS is proven to be bio-compatible and has also been used for the fabrication of implantable biological and surgical equipment. PDMS is a polymer that has both these properties of being bio-compatible and conductive [4, 5, 17]. PDMS in its intrinsic form is less conductive thus to increase its conductance it is doped with various materials like CNT, tin, silver, gold, etc.

1.1 Use of Comsol

The Comsol Multiphysics was used to simulate the working of the electrode. The piezoelectric device physics was used to evaluate the displacement created and the potential generated due to piezoelectricity of PDMS. The potential created due to the flow of bio-signals between neurons results in the deformation of the first PDMS layer due to anti-piezoelectric effect which results in potential being conducted by the subsequent metal layers of gold and titanium, which also provides the electrical contact for the external circuit. The outer PDMS layer serves the role of covering this setup and also acts as the substrate for fabrication process.

The library had the PDMS material that was selectedin Comsol simulation tool with properties defined to behave as an electrode for which four different layers were created for illustrating piezoelectric property. The electrode consists of 4 layers, the first layer is made of PDMS layer of thickness 130µm, second layer is of titanium metal which is deposited using Physical Vapour Deposition (PVD) to a thickness of 40µm this layer improves the adhesion of gold layer which is the third layer, the thickness of this layer is 50µm, the fourth layer is made of higher conductive PDMS and is of 100µm in thickness. The structure of the electrode used for the purpose of simulation in Comsol. The fourth layer is the one that is in contact with the skin while the first layer is the exterior one and acts as a cover and a substrate for the process of PVD. It is the layer from which electrical contact originates for the subsequent connection to the signal conditioning circuit and the oscilloscope for viewing the obtained waveforms.

Further work can be taken through fabrication process for different analysis performed on it such as Potential variation, electric field variation and the charge density created due to piezoelectric property of the PDMS for material properties that can be used in biomedical application that was simulated in Comsol Multiphysics.Using Comsol, the PDMS based electrodes were simulated and the result of their electrical behaviour on deformation is thus found out. These results are very important to determine the response of the material electrode with respect to mechanical and electrical behaviour. The behaviour could be expected when fabricated and can be compared with the performance of the simulated results with that of fabricated. There by its gives imminence pleasure to carry out simulation for understanding the material behaviour even before procurement of chemicals during fabrication. The other advantage of simulating the material property is with respect to the designing of the testing circuit for recording the biomedical signal even before the electrodes are fabricated.

2. Material Properties: PDMS

Polydimethylsiloxane (PDMS) having the chemical formula $(C_2H_6OSi)_n$ belonging to a group of polymeric organo-silicon compounds that are commonly referred to as silicones. PDMS is optically clear, inert, non-toxic, and non-flammable. Its structure is as shown in fig.1. Its applications range from contact lenses and medical devices to elastomers. It gives good elasticity [16] which serves well for instance in applications involving bending or twisting or both, such as micro fluidics. Its permeability is advantageous for instance in gas separation membranes, artificial skin coatings for burns, soft contact lenses or oxygenators in microfluidic analytical devices. The contact angle [16] is a crucial property not only for bonding of the structure, but also for capillary driven devices and it also affects the level of adsorbance. The excellent conductivity of also makes itself an ideal candidate for the suitable filler of conductive polymers. It has the excellent adherence and adaptability to the polymeric substrate and has outstanding antimicrobial property [17] to retard bacterial colonization and reduce the incidence of infections.

Comsol tool is used to successfully develop this material on a virtual environment, so that its behaviour and properties can be studied. Some of the properties of PDMS that have been used in simulation and their typical values are tabulated [16] in table 1. Taking all these properties such as biocompatibility and conductivity into account, this has been the choice of material for the design of electrode used for biomedical applications.

Table 1. Properties of PDMS

Property	Value
Young's modulus	100 kPa to 3 MPa (Based on ratio of Sylgard 184 & elastomer curing agent)
Viscosity	110 cSt
Specific gravity	1.03
Electrical conductivity	0.25×10^{-13} (mho)
Dielectric constant	2.3-2.8
Some of the dopants used	CNT, Copper, Ag, Tin, Nickel

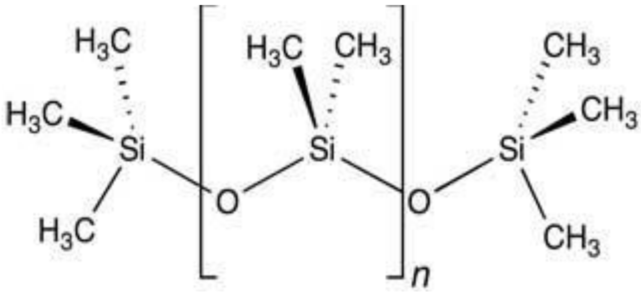

Figure 1: *Structure of PDMS*

The chemical structure of PDMS is shown in figure 1 having properties as listed below

a. PDMS is transparent at optical frequencies (240 nM – 1100 nM), which facilitates the observation of the contents visually or under the microscope,
b. PDMSis basically deformable, which allows the integration of microfluidic valves using the deformation of the channels.

3. Design and Simulation using Comsol Multiphysics

COMSOL Multiphysics is a finite element analysis, solver and Simulation software / FEA Software package for various physics and engineering applications, especially coupled phenomena, or multi-physics.

The Comsol Multiphysics 4.2[7, 8, and 9] was used to simulate the working of the PDMS electrode. The piezoelectric device physics was used to evaluate the displacement created and the potential generated due to piezoelectricity of PDMS. The potential created due to the flow of bio-signals between neurons results in the deformation of the first PDMS layer due to anti-piezoelectric effect which results in potential being conducted by the subsequent metal layers of gold and titanium, which provides the electrical contact for the external circuit. The outer PDMS layer serves the role of covering this setup and also acts as the substrate for fabrication process.

3.1 Electrode Design

In order to create the electrode, a 3D model is selected from the Model Wizard. The electrode consists of 4 layers, the first layer is made of PDMS layer of thickness 130µm, second layer is of titanium metal which is deposited using Physical Vapor Deposition (PVD) to a thickness of 40µm this layer improves the adhesion of gold layer [4] which is the third layer, the thickness of this layer is 50µm, the fourth layer is made of higher conductive PDMS and is of 100µm in thickness[13]. Figure 1 shows the structure of the electrode used for the purpose of simulation in Comsol.

The first layer which is PDMS is selected from the Material Browser and its Parameters can be changed in order to obtain a layer of the desired thickness. The Linear Elastic Material Model node can be used to set the Mechanical Properties of PDMS, such as Young's Modulus to the specified values. The values of other mechanical and electrical properties too are set. Then, layers of titanium and gold are deposited over it. The fourth layer is the one that is in contact with the skin while the first layer is on the exterior and acts as a cover and a substrate for the process of PVD. It is the layer from which electrical contact originates for the subsequent connection to the signal conditioning circuit and the oscilloscope for viewing the obtained waveforms.

This is how the basic electrode design is carried out using Comsol, where the PDMS material is easily simulated with the help of the software.

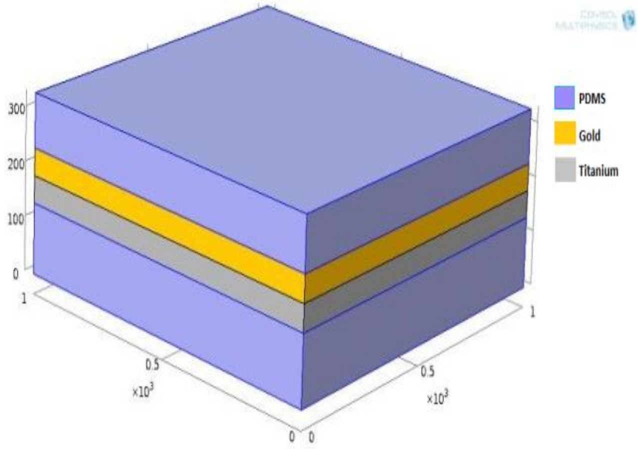

Figure 2: Structure of the dry electrode used for simulation.

3.2 Comsol Procedure for PDMS

The proposed structures is modelled and simulated in COMSOL Multiphysics simulation software. PDMS module was used to design sensor for biomedical applications. In designing the electrode, it consists of three materials, PDMS, titanium and gold. COMSOL simulations were performed on the electrode to investigate the effect of variations in the electric field Vs deformations. We observed the charges that were generated on the outer surface. Using the Comsol Model Builder, we virtually set the deformation levels and observed the corresponding voltage changes. In practical biomedical sensor application this is analogous to the deformation caused in the PDMS sensor due to the variations in the human signals which will result in the charges on the material surface. This surface charge density can be utilized to read the desired signal

3.3 Methodology

The piezoelectric model was applied to all the layers of the electrode, the metal layers were further added to linear elastic model for the purpose of maintaining linear variation as the surface of underlying PDMS surface is varied. The shorter boundaries on either side were added to fixed constraints as they will be adhered to the skin while used in practical usage. Using Comsol Multiphysics tool, a fixed displacement was applied to the layer in contact with the skin and the potential, the charge created on the surface was analyzed, the variation of the electric field throughout the bulk of the electrode material was obtained.

3.4 Working

Whenthe electrode is used in actual practice to sense bio-potentials, the PDMS layer in contact with the skin undergoing deformation results in generation of potential due to anti-piezoelectric effect that has been simulated using Comsol multi physics tool. Using the Comsol Multiphysics tool, a deformation can be simulated. Under the Model Builder, one can select the amount of deformation required and the corresponding voltage developed can be found. Thus, using Comsol Multiphysics, a piezoelectric effect can be simulated. Fig.3 depicts the result obtained for a displacement of 5µm along the z-axis. The potential is highest at the fixed ends of the electrode as maximum stress is felt at these points. Here for a maximum displacement of 5µm, the potential developed is about 20pV.

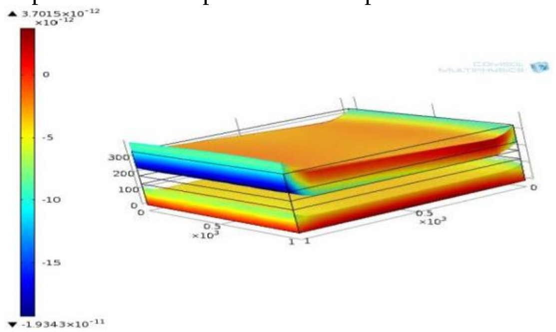

Figure 3: *Deformation (µm) versus Potential (V) generated in the electrode specimen for 5um displacement.*

The variation of electric field inside the bulk of the electrode has been simulated and the same is depicted in fig.4. The maximum electric field is about 300nV/m at the points where the potential is high, and this goes on decreasing towards the outer PDMS layer.

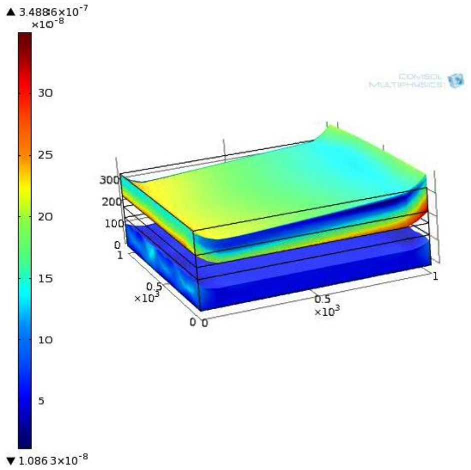

Figure 4: *Deformation (µm) versus Electric field (V/m).*

This electric field results in the generation of free charges in the outer PDMS layer. And the maximum value of surface charge density is $1.2011 \times 10^{-27} C/m^2$. This has been simulated and is depicted in fig.5.

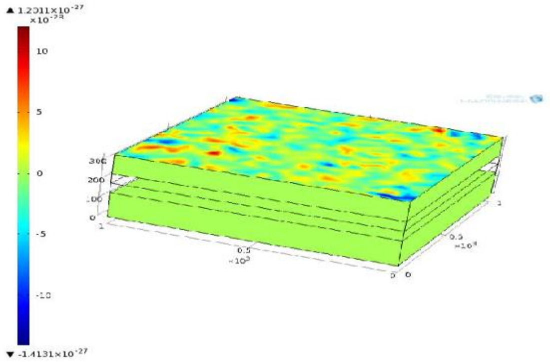

Figure 5: *The charges generated in outer PDMS layer.*

4. Results

The material was synthesized and simulated using Comsol multi-physics tool. The variation of electric field inside the bulk of the electrode has been simulated and values for maximum electric field and surface charge density for displacement of 5um with dimensions of 10mm x 15mm area are listed below in table 2.

Table 2: Parameters and their simulated values

Parameter	**Maximum Value for 5µm deformation**
Potential	20pV
Electric field	300nV/m
Surface charge density	$1.2011 \times 10^{-27} C/m^2$

5. Conclusion

The work describes the behaviour of PDMS based dry electrode when used for measuring bio-potentials, as simulated and developed using Comsol Multiphysics tool. The maximum values of potential, electric field and surface charge density for a deformation of 5µm is tabulated in table 2. PDMS gives approximately the same results as that given by PVDF electrodes. PDMS is found to be more flexible and cost effective. Thus this provides an alternative means to measure essential bio-potentials and also overcomes the inherent limitations of conventional wet electrodes and PVDF. We can thus conclude that PDMS is a good alternative to the present electrodes due to its properties, as seen using the Comsol tool.

6. Future Work

From the obtained simulation results it is clear that the PDMS based electrodes can be used to replace conventional electrodes but as the results show that the voltage levels are of the order of micro/ millivolts, signal conditioning circuit is to be used along with these electrodes to make it work with the existing methods used for acquisition of bio-medical signals.

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