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Simulation and Optimization of stacked PVDF Membrane for Piezoelectric Application

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Abstract: In this paper, a comparative analysis of multilayer stacked PVDF thin film fabricated using two different techniques namely electrospinning and spin coating has been done. The simulation is carried out in COMSOL Multiphysics version 5.0 and the results are analyzed. PVDF is used as the fundamental material in the composition of the structure. The main properties that contribute to the comparative analysis are as follows: displacement, stress, acceleration, and electric potential. for a given material, all the properties are evaluated for a range of frequency. The variance of the properties for the same material under different fabrication techniques is evaluated and analyzed. The study provides comprehensive coverage of spin coating and electrospinning techniques and aims at understanding which technique can be adopted to enhance the efficiency and obtain the desired results.

Keywords : acceleration, displacement, electric potential, stress

INTRODUCTION

There are several methods that can be adopted for the fabrication of thin films onto the desired substrate material considering that the substrate surface is flat. Spin coating is one such technique. A standard process involves depositing a small puddle of a fluid resin onto the center of the substrate. Then the sample is made to spin at very high speed (usually around 3000 rpm). The presence of Centrifugal force will lead the resin to spread and as a result once it reaches the boundary of the sample it falls off the edges of the substrate. The result of this process is a thin film of resin which is formed on the surface. Final film thickness and other properties of the film formed depend on the type of the resin used and its parameters such as viscosity, drying rate, percent solids, and surface tension amongst the other parameters chosen for the spin coating process. The resin is left to rotate until the thin film has achieved the desired thickness for the application chosen.

There is simultaneous evaporation of solvent as the solvent considered is usually volatile in nature. So it can be concluded that the higher the angular speed of spinning, the thinner the film we will get. Also, the thickness of the film depends majorly on the concentration of the solution and the solvent taken for the study. Spin coating is usually employed for the fabrication of those thin films whose thickness has considerably low values. While electrospinning is a fiber production method. The method of electrospinning uses electric force to draw the charged threads of polymer solutions or polymer melts up to desired diameters and length as per the requirements of the study. According to study the Electrospinning process is a voltage-driven process which is governed by the electrohydrodynamic phenomena. A reservoir containing a solution, a pump, a high voltage power source, and a collector contribute to the most basic setup.PVDF is used in the processing of material of both the processes. This study is a descriptive compilation of two processes namely spin coating and electrospinning, aimed at equipping potential users of this thin film deposition technique with the requisite knowledge to enhance better results.

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I. THEORY

A. *Piezoelectric effect*

Some materials were seen to showcase the piezo effect. It can be understood as the generation and accumulation of electric charge when mechanical stress is applied to the material. Accordingly, the materials that obey and exhibit this property need to be dielectric and hence are required to have a crystal symmetry that seems to lack a center of symmetry. An additional necessary constraint is that the material should inherently possess dielectric property. There are numerous examples of Piezoelectric materials, some are natural and some are synthetic crystals and ceramics. But it is evident that some biological matter such as DNA showcases the property of piezoelectricity. Applications of Piezoelectric materials are found in scientific applications and also in everyday civilian life. For instance scanning probe microscopes and everyday applications like a lighter.

B. *Equations for Piezoelectric effect*

The following Piezoelectric Coupling Equations can be used for understanding the concept of the piezoelectric effect.

The equation for Direct piezoelectric effect is given in equation 1

$$V=sF.P+d.F \qquad \text{(Eq1)}$$

The equation for converse piezoelectric effect is given in equation 2

$$D=\varepsilon P.F+d.P \qquad \text{(Eq2)}$$

Herein,

D is a vector for the electric displacement of given piezoelectric material.

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P is a vector for stress for the given piezoelectric material
sF is coefficients of the elasticity matrix for given piezoelectric material at constant electric field strength,
V is a vector for strain for the given piezoelectric material
εP is dielectric matrix coefficients for given piezoelectric material at constant mechanical strain
F is a vector for the electric field for the given piezoelectric material
d is a direct or converse piezoelectric effect for the given piezoelectric material

The generation of varying amounts of stress in the piezoelectric materials can be seen in the application of electric fields in different directions on the constructed structure. The coefficient is used along with sign conventions which causes the applied field to be zero down. For determining the direction, the axes are numbered as 1, 2, and 3 and so on which is in accordance with axes labeled *x*, *y*, *and z*. Also, polling is to be projected in the direction of the axis labeled as 3 always. Electrical and mechanical characteristics are inferred with the help of coefficients with double subscripts wherein the first subscript describes the electric field direction with reference to the voltage applied or charge produced. The mechanical stress direction is denoted by the second subscript.

The electromechanical coupling coefficient exists in two forms. The first form being the actuation term d and the second form being the sensor term g. The piezoelectric coefficients along with their notations can be explained with $d33$.

Where,

d denotes stress applied in the third direction. *3* denotes axis 3 is perpendicular to electrodes. *3* denotes a constant of piezoelectricity.

II. SYSTEM DEVELOPMENT

The predefined multiphysics interfaces in COMSOL Multiphysics version 5.0 combine the needed relevant physics governing the equations through structured laws which are also known as boundary conditions. Hence they provide a good starting point for setting up more complex multiphysics problems that involve materials that are piezoelectric in nature.

A. *Methodology adopted*

In COMSOL Multiphysics version 5.0 it has the option of transparent workflow, this allows us to visualize the constituent physics interfaces and helps to comprehend a simplified version of the constructed design. There is also a separate Multiphysics node which lists out how the different physics interfaces are related to one another. The type of mesh chosen for the COMSOL Multiphysics simulation strongly affects the designs' modeling time and requirements. So, one of the most important memory-intensive steps is meshing. The right type of meshing helps in solving a finite element problem in the design while compiling. Choosing the right mesh for the designed model involves the procedure of choosing the correct element type and also the correct element size. Here for both the spin coating structure and the electrospinning structure the mesh was chosen as normal as when it was set to fine or extremely fine the computation time was increasing ineluctably.

B. *Experimental details*

The block diagram, shown in Fig. 1, depicts the geometry of structures of both the spin coating process and the electrospinning process.

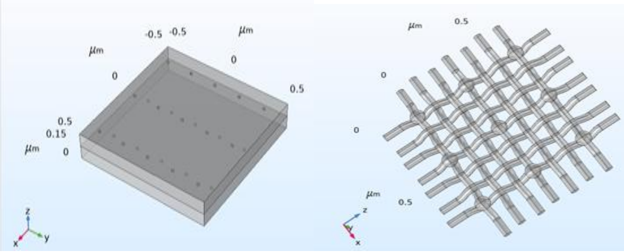

Fig. 1: Geometry of spin coating and electrospinning

In the spin coating structure, the below block consists of PVDF and the spheres in it represent the silver dopants. The top layer block consists of PVDF and the spheres in it are a combination of the chosen two dopants. In the electrospinning structure, the fibers are made of PVDF material with spheres embedded in between which represent the combination of the chosen dopants. The linear elastic material, fixed constraints, ground, and the boundary load are set for both structures. The mesh is set as normal and the structure is built.

The structure is computed for two studies that are eigenfrequency and for frequency domain. In eigenfrequency, the manual search method is chosen and the desired number of eigenfrequencies is set as six with the unit of Hz. The eigenfrequency search method around the shift is set as closest in absolute value. In the frequency domain, the frequency range is set as starting at 435Hz and stopping at 1870 Hz with a step size of 200. These two study domains are then computed in the COMSOL Multiphysics software to yield the consolidated structure with the desired parameters which are free of errors. The plots for stress (Von Mises), displacement, acceleration(surface), and the electric potential can be found under the result section in COMSOL by setting the appropriate parameter for each property.

III. RESULT AND DISCUSSION

A. Structural Analysis

The COMSOL Multiphysics version 5.0 software incorporates the predefined physics interfaces that have precisely designed settings for the structural framework development and evaluation. The Structural Mechanics Module includes built-in material models to choose from. It also caters to the ability to enter user-defined data for the material models which can be altered based on the type of evaluation being conducted. It is also possible to enhance the dimensions of the geometry and also the properties of the materials for the developed design with the add-ons present under the Optimization Module in Comsol Multiphysics version 5.0.

B. Analysis of Results

COMSOL multiphysics selects by default a scale factor for the deformation making sure that any deformation is evident. In the plots, the actual properties can be understood when looking at the color of the plot and comparing it to the scale on the right. If the frequency is varied the properties change accordingly which is seen as a change in the values on the scale.

a.) Displacement

Materials exhibiting piezoelectric properties yield displacement. They can also be used to produce forces. Force generation and a reduction in displacement are coupled. The force of the highest magnitude that can be generated in a piezoelectric material is directly proportional to the maximum displacement and material stiffness. At maximum force generation, displacement drops to zero.

$\Delta L = F\,k$

k is material stiffness ΔL is displacement

F is force

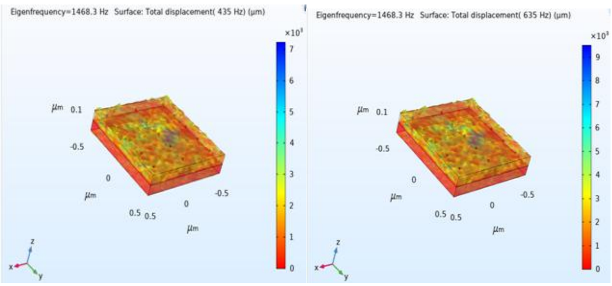

Fig 2: 3D displacement plot for spin coating

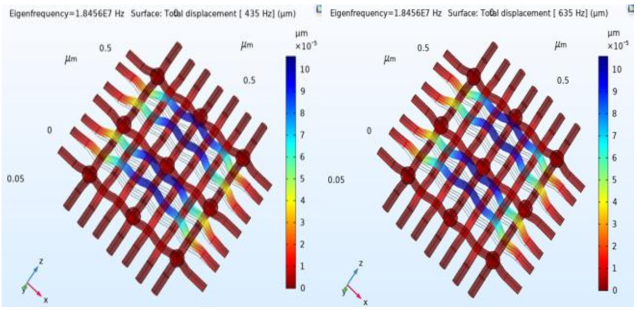

Fig 3: 3D displacement plot for electrospinning

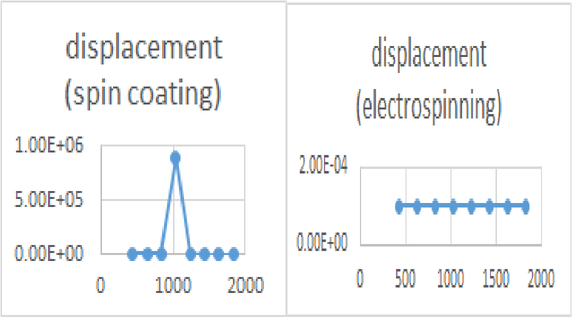

Fig 4: Displacement vs frequency plots

b.)Von Mises stress

As stress is a tensor, it is proven to be difficult to plot the same therefore in the result section, all the stress plots shown are Von-Mises stress. This stress is derived from the Von-Mises yield criterion. This states that the yielding of material starts at a particular designated value of this stress. The Von-Mises stress($\square_{\square\square\square}$) is defined as

$$\square^2_{\square\square\square} = \frac{1}{2}\Big[(\square_{11} - \square_{22})^2 + (\square_{22} - \square_{33})^2 + \square 33 - \square 112$$

$$+6\left((\square_{12})^2 + (\square_{23})^2 + (\square_{31})^2\right)\Big]$$

Where $\square_{\square\square}$are the components of the stress tensor.

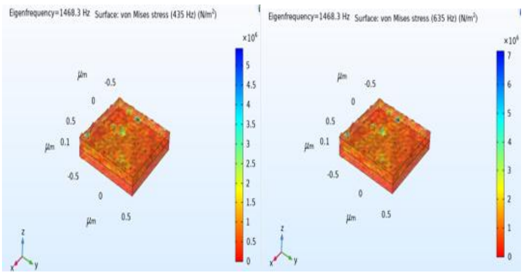

Fig 5:3D Von-Mises stress plot for spin coating

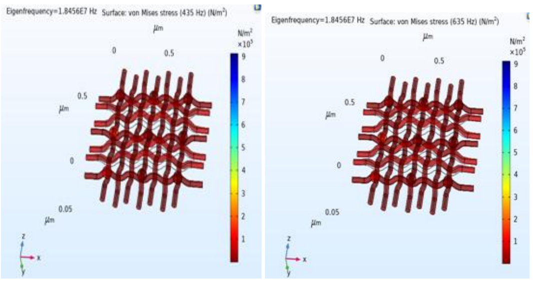

Fig 6:3D Von-Mises stress plot for electrospinning

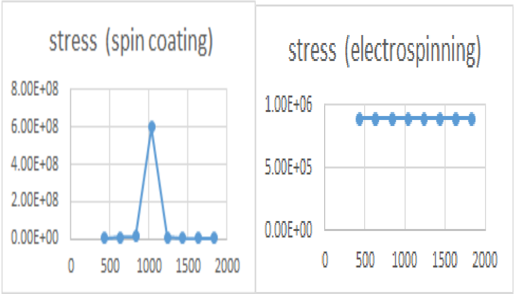

Fig 7: Von-Mises stress vs frequency plot for electrospinning

c.)Surface acceleration

The piezoelectric material is spring-loaded with a seismic mass in contact with a crystal, when subjected to an acceleration, the seismic mass stresses the crystal to a force accounting for a voltage generated across the crystal. The forces generate an output voltage corresponding to the acceleration.

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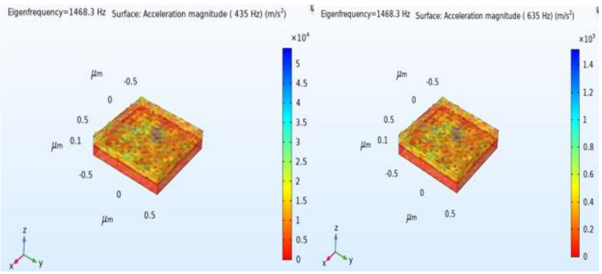

Fig 8: 3D surface acceleration plot for spin coating

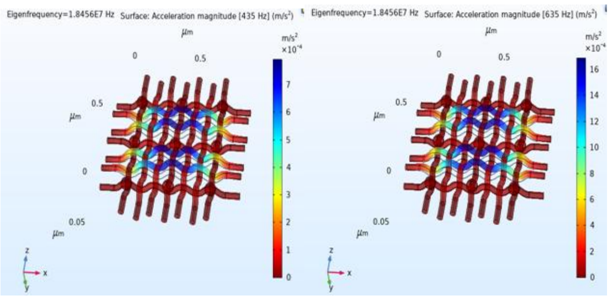

Fig 9: 3D surface acceleration plot for electrospinning

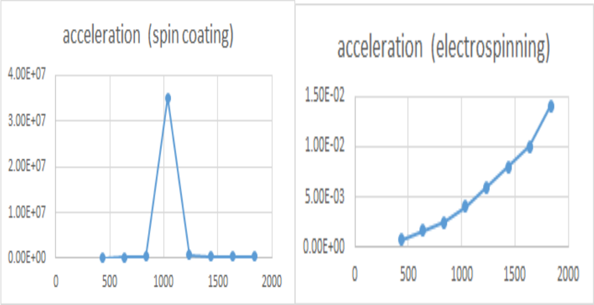

Fig 10: surface acceleration vs frequency plot

d.)Electric potential

In a piezoelectric material, when a given amount of force is applied in order to stretch or bend it, it is seen that an electric potential will be generated. But on the contrary, when an electric potential is applied, the piezoelectric material undergoes a deformation i.e. the piezoelectric material is extended or bent.

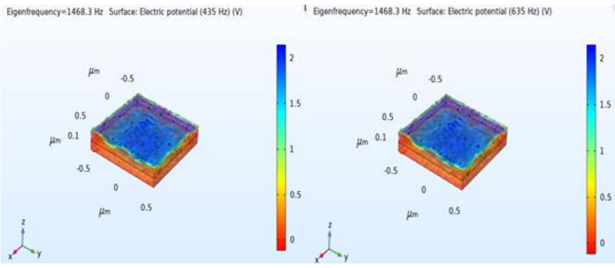

Fig 11: 3D electric potential plot for spin coating

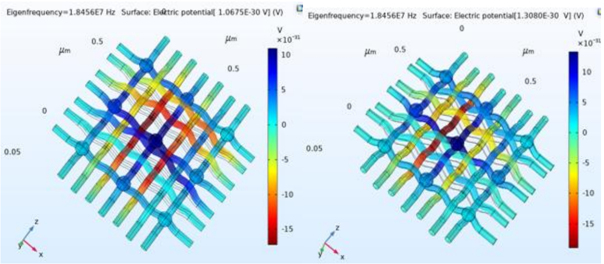

Fig 12: 3D electric potential plot for electrospinning

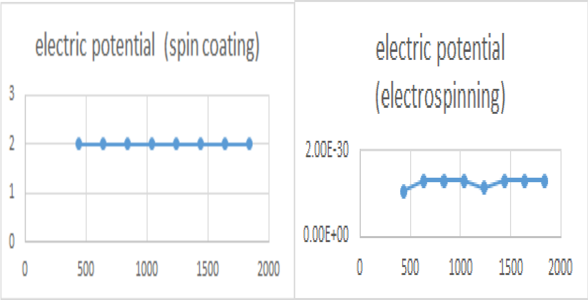

Fig 13: electric potential vs frequency plot

IV. CONCLUSION

The conceptual knowledge of electrospinning and spin coating techniques has been understood and their structural models are implemented through simulation which facilitates the description of the process for material systems of different material combinations, which vary in their characteristics. The materials that were used are Copper, Molybdenum, Cobalt, Selenium, Copper Selenide, and Bismuth. PVDF is a vital component in the framework of the structure. It has a low density and a glass transition temperature (Tg) of about -35 degrees celsius and is predominantly 50-60% crystalline in nature. When poled it is observed through various studies that PVDF is a polymer exhibiting ferroelectric properties that shows efficient piezoelectric properties. These very characteristics make it essential to function as sensors and also in various other battery applications. PVDF is observed to have a negative □$_{33}$ value. As a result of which the material will experience compression instead of expansion or expansion instead of compression when exposed to the same electric field or electric potential. The basic principles that govern the process such as stress (Von Mises stress), displacement, acceleration (surface), and electric potential are strongly emphasized. This will aim to educate current researchers in the field of thin-film fabrication, to facilitate and enhance the better exploitation of both these techniques.

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Dr. G Shireesha has a M.Sc, M.Phil and Ph.D accredited to her name. She has 22 years of teaching experience as an Assistant Professor in R V College of Engineering in the department of Physics. She is passionate in the field of Thin Films and Polymer Nanocomposites. She has published various papers in international journals and conferences in the same field.