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Mathematical model to predict the characteristics of polarization in dielectric materials: The concept of piezoelectrcity and electrostriction

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A B S T R A C T

Model was developed for the prediction of polarization characteristics in a dielectric material exhibiting piezoelectricity and electrostriction based on mathematical equations and MATLAB computer simulation software. The model was developed based on equations of polarization and piezoelectric constitutive law and the functional coefficient of Lead Zirconate Titanate (PZT) crystal material used was 2.3×10^{-6} m (thickness), the model further allows the input of basic material and calculation of parameters of applied voltage levels, applied stress, pressure, dielectric material properties and so on, to generate the polarization curve, strain curve and the expected deformation change in the material length charts. The mathematical model revealed that an application of 5 volts across the terminals of a 2.3×10^{-6} m thick dielectric material (PZT) predicted a 1.95×10^{-9} m change in length of the material, which indicates piezoelectric properties. Both polarization and electric field curve as well as strain and voltage curve were also generated and the result revealed a linear proportionality of the compared parameters, indicating a resultant increase in the electric field yields higher polarization of the dielectric materials atmosphere.

Capsule Summary: Mathematical model was developed and employed for the prediction of polarization in dielectric materials using the concept of piezoelectrcity and electrostriction. Electric field effects on the polarization of the dielectric materials, as well as results revealed the change in length of the dielectric material demonstrating piezoelectric characteristics of the PZT crystal material.

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INTRODUCTION

A dielectric is an electrical insulator that can be polarized by an applied of an electric field. When a dielectric is placed in an electric field, the process or the system do not allow the electric charges to flow through the material as they do in an electrical conductor but only slightly shift from their average equilibrium positions may cause dielectric polarization. In this system because of dielectric polarization, positive charges are displaced in the direction of the field and negative charges shift in the opposite direction. This creates an internal electric field that reduces the overall field within the dielectric itself. If a dielectric is composed of weak bond molecules, in this case, these molecules not only become polarized, but also reorient so that their symmetry axes align to the field (Amjad et al., 2019; Costa et al., 2019; Das and Choudhary, 2019; Liu et al., 2019; Sharma et al., 2019; Xie et al., 2019; Xu et al., 2019). Research conducted on the insulator revealed that low electrical conduction and dielectric materials with a high polarizability posse the latter which is expressed by a number called the relative permittivity. The insulator is generally use to indicate electrical obstruction while the dielectric is use to indicate the energy storing capacity of the material (by means of polarization). A common example of a dielectric is the electrically insulating material between the metallic plates of a capacitor. The polarization of the dielectric by the application of electric field increases the capacitor's surface charge for the given electric field strength as reported by Herrera (2014).

The research work conducted on dielectric material with zero electrical conductivity which revealed exhibiting only a displacement current as well as store and return electrical energy as if it were an ideal capacitor. Dielectric substance show various characteristics based on their chemical, physical and mechanical composition, whereas the characteristics of the electrostriction, piezoelectricity, ferroelectricity and pyroelectricity was reported by Dahiya and Valle (2013).

Investigation carried out revealed that electrostriction is a property of all dielectrics that causes change in shape material under the application of an electric field. Electrostriction is a property of all dielectric materials, and is caused by a slight displacement of ions in the crystal lattice upon being exposed to an external electric field. In this case, positive ion was displaced in the direction of the field, while negative ion was displaced in the opposite direction. This displacement will accumulate throughout the bulk material and result in an overall strain (elongation) in the direction of the field and the thickness material will be reduced in the orthogonal directions characterized by Poisson's ratio. All insulating materials consisting of more than one type of atom was ionic to some extent due to the difference of electronegativity of the atoms, and therefore exhibit electrostriction (Cordero, 2015). The resulting strain (ratio of deformation to the original dimension) was observed to be proportional to the square of the polarization. Reversal of the electric field does not reverse the direction of the deformation Frederic as reported by Christians (2002). Electrostriction is the fundamental electromechanical coupling in all materials, since all materials possess atoms, ions, molecules, or domains that are either polarized or polarizable, application of an electrical excitation (field or induced polarization) distorts the charge distribution, which is then coupled to distortion of the actual dimensions. In short, elastic strain in the material resulted from distortion of the bond lengths, bond angles, electron distribution functions, or electric dipoles with an applied electric stress (Erol et al., 2019; Gaikwad et al., 2019; Gareeva et al., 2019; Jin et al., 2019; Kumar and Sarangi, 2019). In present investigation, model prediction for the characteristics of polarization in a dielectric material exhibiting piezoelectricity and electrostriction was developed and employed for the monitoring, prediction and simulation using derived mathematical equations as well as MATLAB computer simulation software.

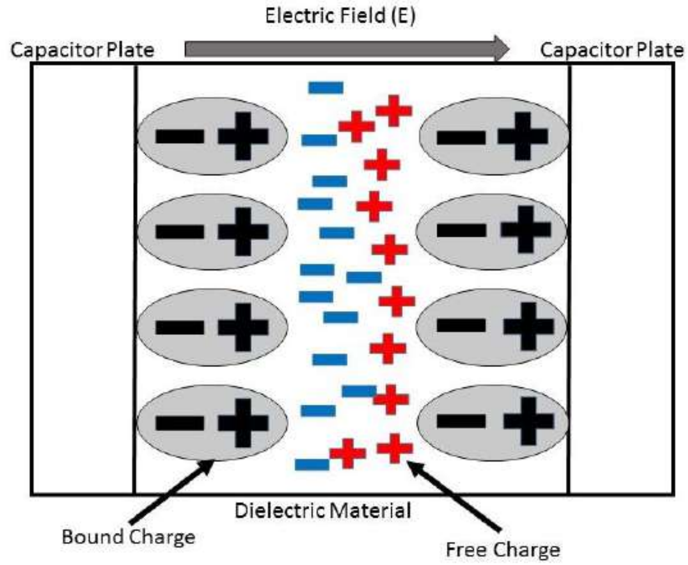

Fig. 1: Dielectric material in a capacitor showing the bound charges-touching the capacitor plates, and the free charges usually floating around in the material, but all aligned due to P is polarization (David, 1999).

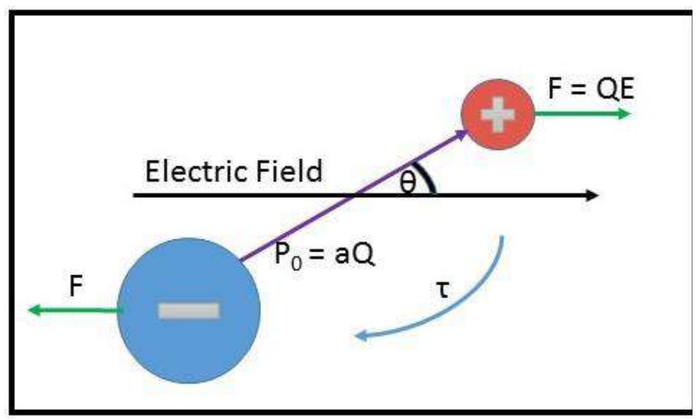

Fig. 2: The effect of an electric field on a typical dipolar molecule. P_0 symbolizes the dipole moment, a is the distance away from the body center of the molecule and F is the force, which is the charge Q, times the electric field, E. (David, 1999).

MATERIAL AND METHODS

This anisotropic effect is described in mathematical tensor form as described in Eq. 1 (Jozef et al., 2004).

$$S_{ij} = Q_{ijkl} \times D_l \quad (1)$$

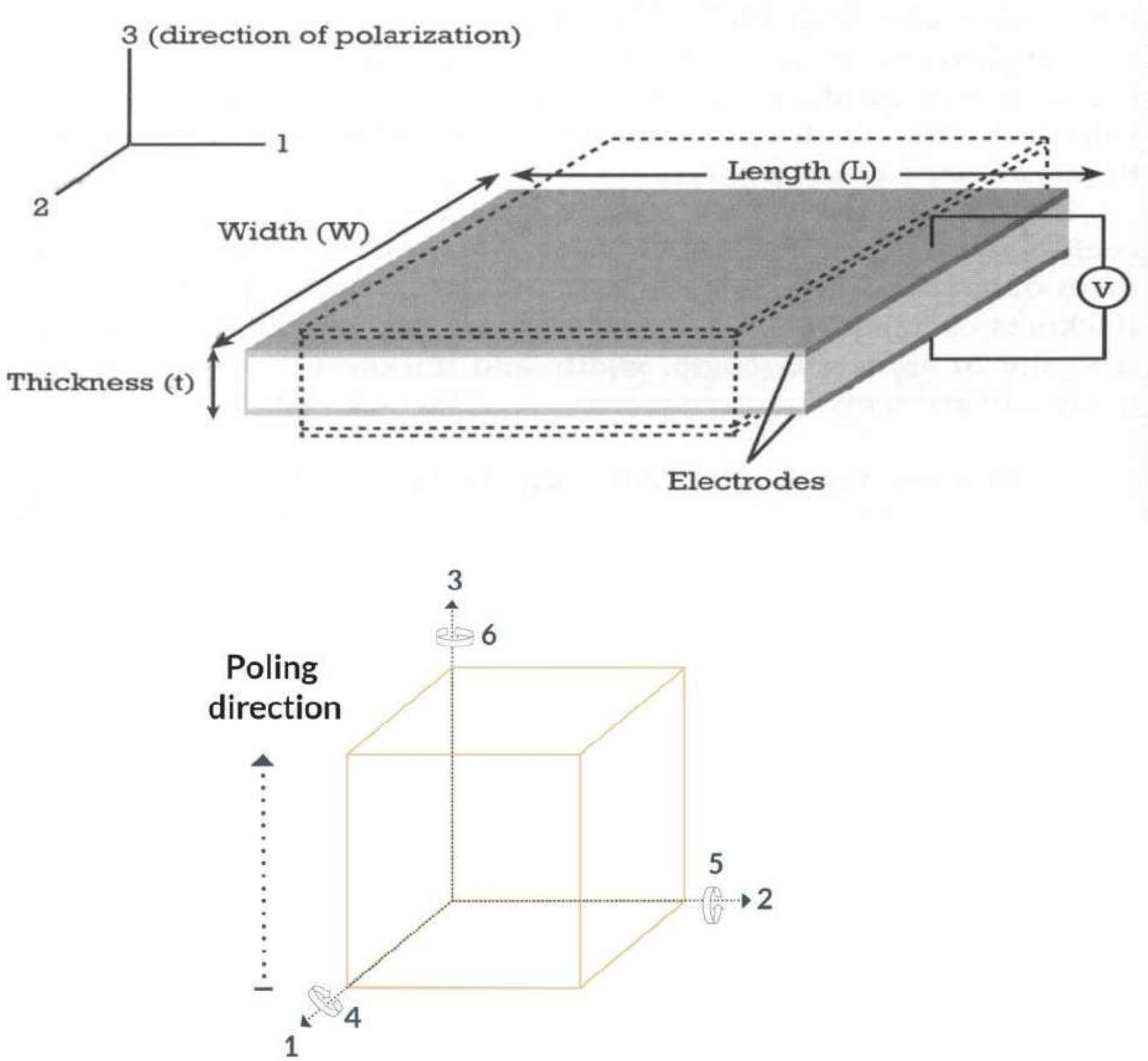

Fig. 3: Sample dielectric material with piezoelectric properties, showing the pooling direction and pressure (strain – Stress) (Clement et al., 1998).

Where, S_{ij} is the strain components (unitless), D_l is the dielectric displacements (C m^{-2}), and Q_{ijkl} is the components of the electrostrictive coefficient (C^2 m^{-4}).

Although all dielectrics exhibit some electrostriction, certain engineered ceramics, known as relaxor ferroelectrics, have extraordinarily high electrostrictive constants. The most commonly used is lead magnesium niobate (PMN), lead magnesium niobate-lead titanate (PMN-PT), lead lanthanum zirconate titanate (PLZT). Piezoelectricity is the electric charge that accumulates in certain solid materials (such as crystals, certain ceramics, and biological matter such as bone, DNA and various proteins) in response to applied mechanical stress. The word piezoelectricity means electricity resulting from pressure and latent heat. It is derived from the Greek word πιέζειν; piezein, which means to squeeze or press, which means amber, an ancient source of electric charge, french physicists Jacques and Pierre Curie discovered piezoelectricity in 1880 (Michael, 2015).

The piezoelectric effect obtained as a result of the linear electromechanical interaction between the mechanical and electrical states in crystalline materials with no inversion symmetry was reported by vaious research groups. The piezoelectric effect is a reversible process in which the materials exhibiting the piezoelectric effect has the internal generation of electrical charge resulting from an applied mechanical force as well as exhibit the reverse piezoelectric effect, the internal generation of a mechanical strain resulting from an applied electrical field can be related to lead zirconate titanate crystals (PZT) which generate measurable piezoelectricity when their static structure is deformed by

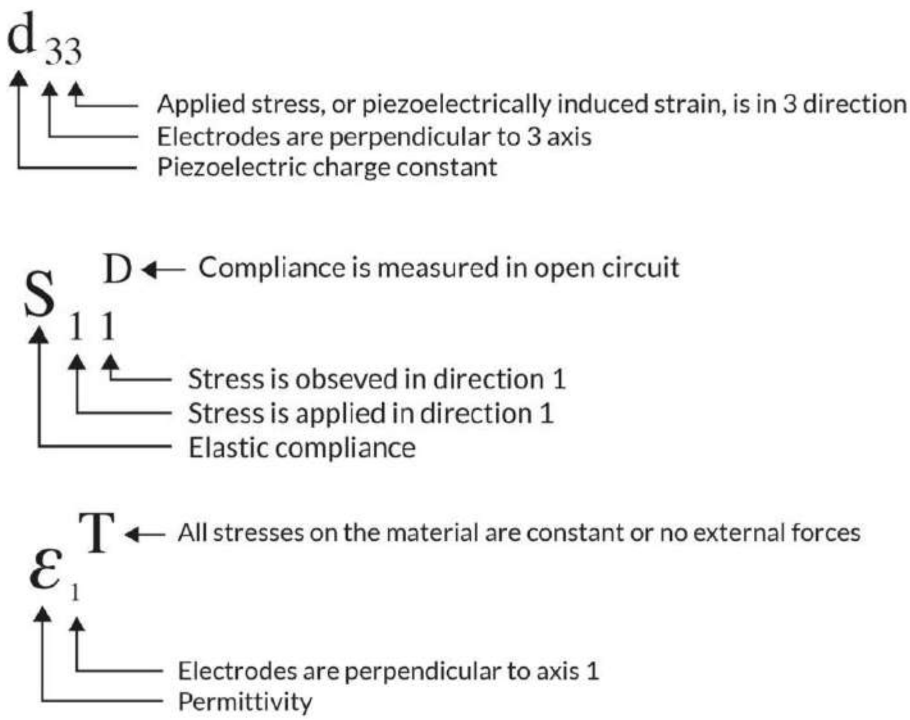

Fig. 4: Piezoelectric constants and their subscripts meaning (Arnold, 2003).

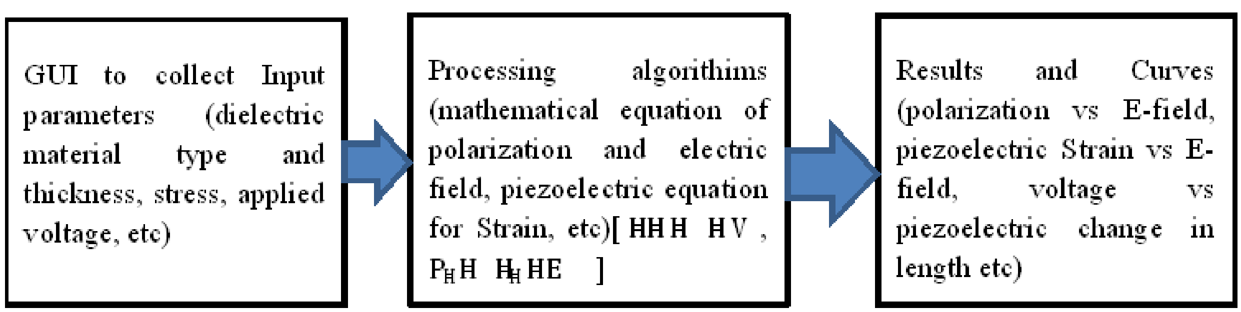

Fig. 5: block diagram of the mathematical model

about 0.1% of the original dimension. Conversely, the same crystals will change about 0.1% of their static dimension when an external electric field is applied to the material. The inverse piezoelectric effect is used in the production of ultrasonic sound waves as reported by Arnold et al. (2003).

The related piezoelectric effect occurs only in a particular class of dielectrics, while electrostriction applies to all crystal symmetries as well as the piezoelectric effect only applies to the 20 piezoelectric point groups. Research conducted revealed that electrostriction is a quadratic effect, unlike piezoelectricity, which is a linear effect Arnold et al. (2003).

Dielectric polarization

Investigation conducted on dielectric polarization revealed that dielectric occurs when a dipole moment is formed in an insulating material because of an externally applied electric field. When a current interact with a dielectric (insulating) material, the dielectric material will respond with a shift in charge distribution which result to the positive charges aligning with the electric field and the negative charges aligning against it as well as by taking advantage of this response, important circuit element such as capacitor can be made to withstand the significance of the effect. A simple illustration was made using a capacitor as an example. The Figure 1 shows an example of a dielectric material in between two conducting parallel plates. The charges in the material will have a response to the electric field caused by the plates. Using the capacitor model, it is possible to define the relative permittivity or the dielectric constant of the material by setting its relative permittivity equivalent to the ratio of the measured capacitance and the capacitance of a test capacitor, which is also equal to the absolute permittivity of the material divided by the permittivity of vacuum, is expressed in Eq. 2.

$$\varepsilon r = \frac{Q}{Q_o} = \frac{C}{C_o} = \frac{\varepsilon}{\varepsilon_o} \quad (2)$$

In some materials whose molecules are permanently polarized by chemical forces, such as water molecules, some of the polarization is caused by molecules rotating into the same alignment under the influence of the electric field. One of the measures of polarization is electric dipole moment, which is equal to the distance between the slightly shifted center of positive and negative charge multiplied by the amount of one of the charge. Polarization (P) expressed in terms of quantitative is the amount of dipole moment *p* per unit volume *V* of a polarized material and the mathematical expression is shown in Eq. 3.

$$P = \frac{p}{V} \quad (3)$$

The representative of atoms, molecules, groups of ordered atoms or molecules (domains), or even macroscopic particles, the dipoles are pictured as opposite charges ±q separated by a vector distance l directed from the negative to the positive charge. Thus, the individual dipoles have moment's p defined as shown in Eq. 4.

$$p = ql \quad (4)$$

Orientational polarization arises when there is a permanent dipole moment in the material. Materials such as HCl and H_2O will have a net permanent dipole moment because the charge distributions of these molecules are skewed. For example, in an HCl molecule, the chlorine atom was negatively charged and the hydrogen atom was positively charged causing the molecule to be dipolarized. The dipolar nature of the molecule will cause a dipole moment in the material, however, in the absence of an electric field; the dipole moment is canceled out by thermal agitation resulting in a net zero dipole moment per molecule. When an electric field is applied however, the molecule will begin to rotate to align the molecule with the field, causing a net average dipole moment per molecule. Force F in Figure 2 is seen as a torque τ acting on the rigid body of the dipolar molecule. Using this model, the equation for the torque is shown in Eq. 5.

$$\tau = (F\sin\theta)a \quad (5)$$

Where, a is direction from the negative to the positive charge. An electric dipole in an external electric field is subjected to a torque (Eq. 6).

$$\tau = pE \sin\theta \quad (6)$$

Where, θ is the angle between p and E. The torque tends to align the dipole moment p in the direction of E. The potential energy of the dipole is shown in Eq. 7.

$$Ue = -pE\cos\theta = -P \cdot E \quad (7)$$

In a non-uniform electric field, the potential energy of an electric dipole also varies with position, and the dipole was subjected to a force. The force on the dipole is in the direction of increasing field when p is aligned with E, since the potential energy *Ue* decreases in that direction.

The polarization of a medium P gives the electric dipole moment per unit volume of the material; it is expressed in unit of coulomb per meter squared. When a dielectric is placed in an electric field, it acquires a polarization that depends on the field.

$$\kappa = 1 + \frac{\chi e}{\varepsilon 0} \quad (9)$$

When an electric field is applied in a dielectric material, the bound charges in the material are separated inducing electric dipole moment. This electric displacement field (D) is defined by Kuzmina et al. (2016) as shown in Eq. 10.

$$D = \varepsilon_0 E + P_{total} \quad (10)$$

Where, E is the applied electric field, ε_0 is the vacuum permittivity and P is the total polarization assuming the polarization is due to linear polarization.

$$P_{total} = P_{linear} = P_l \quad (11)$$

But Polarization due to linear displacement is defined as shown in Eq. 12.

$$P_l = \varepsilon_\circ \chi E \quad (12)$$

Where, χ is the electric susceptibility of the dielectric which is related to the relative permittivity of the material as shown in Eq. 13.

$$\varepsilon_r = 1 + \chi \quad (13)$$

Therefore, the displacement field, D is shown in Eq. 14.

$$D = \varepsilon_\circ E + \varepsilon_\circ \chi E \quad (14)$$

The electric displacement filed is equal to the surface charge density (s) which is defined as charge per unit surface area (Eq. 15).

$$D = \sigma = \frac{Q}{A} \quad (15)$$

Piezoelelctric polarization

Table 1: The values of modeling parameters

Parameters	Value	Unit
Piezoelectric strain constant, d	390×10^{-12}	CN^{-1}
Stress, T	5	Nm^{-2}
Elastic compliance, s	0.1923×10^{-10}	m^2/N
Piezoelectric voltage constant, g	2.4×10^{-3}	m^2/C (VmN^{-1})
Youngs modulus, Y	5.2×10^{10}	$N\ m^{-2}$
Material thickness, th	2.3×10^{-6}	m
Permittivity of free space, ε_0	8.8541×10^{-12}	Fm^{-1}

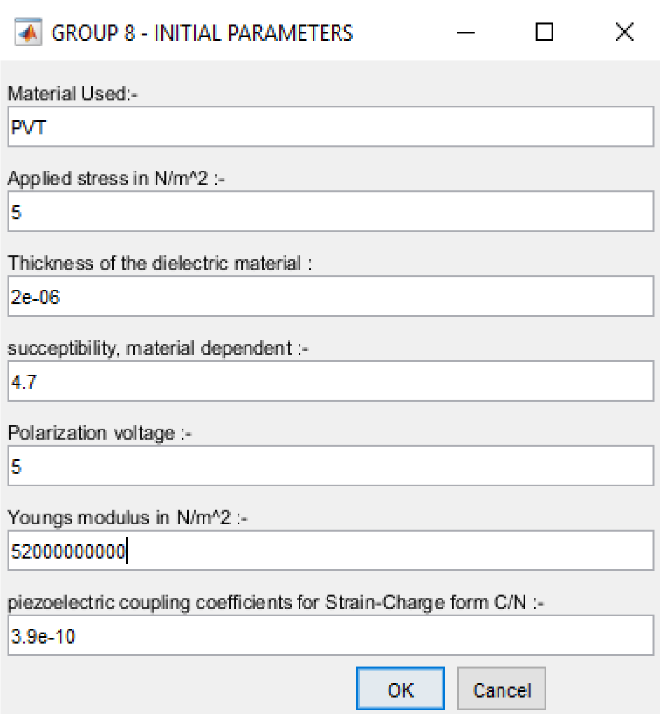

Fig. 6: Required start up parameters

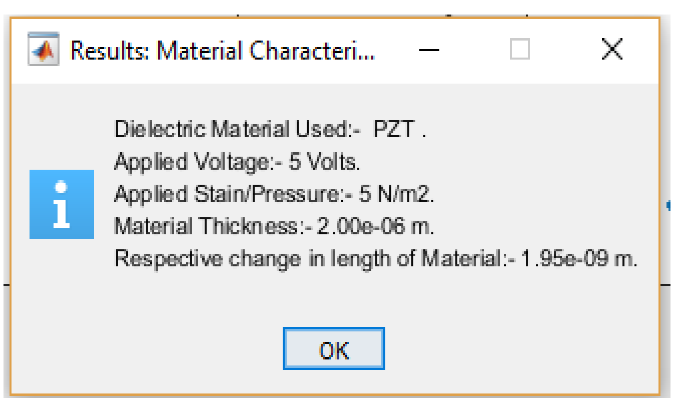

Fig. 7: Result dialogue box displaying predicted information

The anisotropic nature of piezoelectric ceramics, properties vary depending on direction. To identify directions in a piezoelectric ceramic element, a specific coordinate system is used. Three axes are defined, termed 1, 2, and 3, analogous to X, Y, and Z of the classical three-dimensional orthogonal set of axes. The polar, or 3 axis, is determined by the direction of the poling. Unless the component needs to be utilized in shear mode, electric field is applied in direction 3. Directions 1 and 2 are physically equivalent, so they can be defined as arbitrarily perpendicular to direction 3 and to each other. The directions termed 4, 5 and 6 correspond to tilting (shear) motions around axes 1, 2 and 3 respectively. In shear mode, after poling, electrodes are stripped and redeposited perpendicular to axis 1. In this case, once electric field is applied, the component shears in one dimension without any change in other dimensions. Piezoelectricity is described mathematically within a material's constitutive equation, which defines how the piezoelectric material's stress (T), strain (S), charge-density displacement (D), and electric field (E) interact. There are different ways of writing the fundamental equations of the piezoelectric materials, depending on which variables are of interest. The two most common forms are (the superscript t stands for matrix-transpose):

$$S = s^E \cdot T + [d]^t \cdot E \qquad S = s^D \cdot T + [g]^t \cdot D$$

$$D = d \cdot T + \varepsilon^T \cdot E \qquad E = -g \cdot T + [\varepsilon^T]^{-1} \cdot D$$

These matrix relationships are widely used for finite element modeling. In relation to other elastic materials, Strain is proportional to the applied stress. But in addition for piezoelectric materials, an additional piezoelectric term is present, relating strain to electric field (Michael, 2015). Piezoelectric materials are characterized by several coefficients. Piezoelectric coefficients with double subscripts link electrical and mechanical quantities. The first subscript provides the direction of the electric field, or the dielectric charge produced. The second subscript provides the direction of the mechanical stress or strain as illustrated in Figure 4.

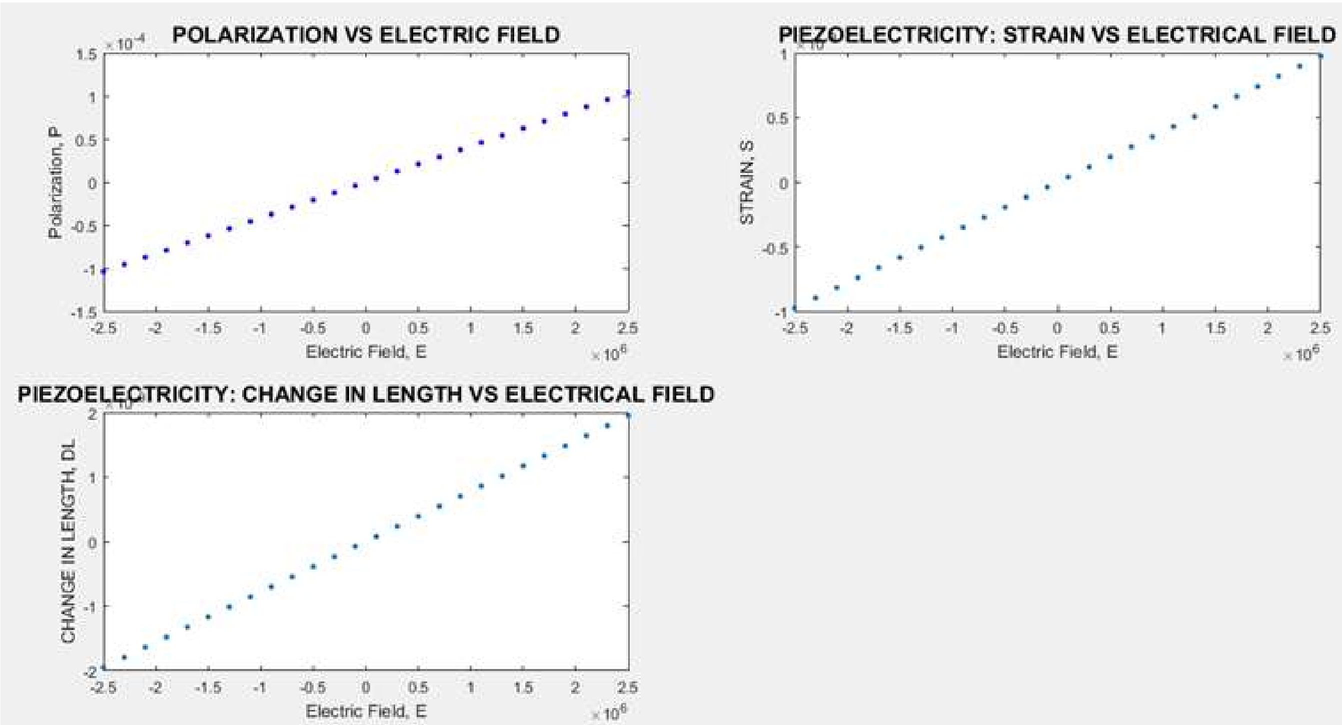

Fig. 8: Output curves showing predicted characteristics

The piezoelectric constants relating the mechanical strain produced by an applied electric field are termed the piezoelectric deformation constants, or the "d" coefficients. They are expressed in meters per volt [m/V]. Conversely, these coefficients which are also called piezoelectric charge constants may be viewed as relating the charge collected on the electrodes to the applied mechanical stress. The units can therefore also be expressed in Coulombs per Newton [C/N].

In addition, several piezoelectric material constants may be written with a "superscript" which specifies either a mechanical or an electrical boundary condition. The superscripts are T, E, D, and S, signifying. Where, T=constant stress=mechanically free, E = constant field=short circuit, D = constant electrical displacement=open circuit and S = constant strain=mechanically clamped. Here are three examples of parameters used in the piezoelectric equations together with an explanation of their notation. The change in length per unit applied voltage can be calculated as shown in Eq. 16.

$$\varepsilon = d\,E \quad (16)$$

But $E = \frac{V}{l}$ where V = applied voltage, l = length of the material, and

$$\varepsilon = \frac{\Delta l}{l}$$

$$\frac{\Delta l}{l} = d\,\frac{V}{l}$$

$$\Delta l = d\,V \quad (17)$$

Design and methodology

The project would be implemented mathematically using the piezoelectric constitutive laws on the Lead Zirconate Titanate, PZT. The implementation would be done using MATrixLABoratory software by Mathworks Incorporated. The model would require key basic parameters on startup to run the system and predict the intended characteristics like Polarization – electric field relationship, strain – electric field relationship, change in length-induced voltage relationship.

The model is designed with the block diagram illustrated in Figure 5

Simulation parameters

As stated, the dielectric material utilized for this project is Lead Zirconate Titanate, PZT and its data is shown in appendix A–PZT data sheet [5], but the basic utilized parameters are tabulated in Table 1. These parameters are inputted into the model using an input dialogue box that specifies the required data. This input method is illustrated in Figure 6. On startup, the dialogue box pops up with default parameters of the PZT crystal as shown in Figure 6, these values are editable and allow for utilization of other

Dielectric materials with piezoelectric properties. It allows a large scale prediction of dielectric properties

RESULTS AND DISCUSSION

The results generated by the model outputs 3 individual curves and a result dialogue box as illustrated in Figure 7 and Figure 8. The dialog box displays the predicted results from the mathematical model after indicating the type of dielectric material used. The applied stress which generates a change in length of 1.95×10^{-9} m. and the Dielectric material used to run the simulation. The curve show a linear slope, Figure 8a demonstrated the polarization verse Electric field showing that as the applied voltage increases, the polarization value also increases, at zero (0) electric field, there is no Polarization. At 1×10^{6} Vm^{-1}, a corresponding polarization value of 0.5×10^{-4} cm^{-2}. Looking at the prediction model for piezoelectricity, tagged figure 8b: strain verses electrical field and 8c: Change in length verse electric field, shows the resultant effect of applied voltage on Strain and change in length of the piezoelectric material.

The relationship between polarization and electric field was examined using the Matlab Compute Programme Language and the results obtained revealed linear increase in polarization upon the influence of electric field as shown in figure 8. The effect of electric field on piezoelectric material in terms of variation in length was observed to be linear in characteristics, indicating that the charge electric field influences the piezoelectric materials. The figure 8 also illustrates that the variation in the polarization, piezoelectric material in terms of strain, length can be attributed to the variation in the electric field.

CONCLUSIONS

The developed mathematical model was able to monitor, predict and simulate the dielectric properties indicating the effects of electric field on the polarization of the dielectric materials, as well as revealed the resultant change in length of the dielectric material demonstrating piezoelectric characteristics of the PZT crystal material. This further proves the possibility of the utilization piezoelectricity in a number of useful applications, such as the production and detection of sound, piezoelectric inkjet printing, generation of high voltages, electronic frequency generation, and everyday uses such as acting as the ignition source for cigarette lighters, and push-start propane barbecues, as well as being used as the time reference source in quartz watches.

REFERENCES

Amjad, T., Sadiq, I., Javaid, A.B., Riaz, S., Naseem, S., Nadeem, M., 2019. Investigation of structural, electrical, electrical polarization and dielectric properties of CTAB assisted Ni^{2+} substituted R-type nano-hexaferrites. Journal of Alloys and Compounds 770, 1112-1118.

Arnold, A., Ehrhardt, M., Sofronow, I., 2003. Descrete transparent boundary condition for the schrodringer equation, fast calculation, approximation and stability. Communication in Mathematical Science 1(3), 501-556.

Cordero, F., 2015. Electric properties and enhanced piezoelectric response at morphotropic phase boundaries, New York, IEEE Press, 210.

Costa, P., Al-Rjoub, A., Rebouta, L., Manninen, N.K., Alves, D., Almeida, B., Barradas, N.P., Alves, E., 2019. Influence of Al/Si atomic ratio on optical and electrical properties of magnetron sputtered Al1-xSixOy coatings. Thin solid films 669, 475-481.

Dahiya, R., Valle, M., 2013. Robotic tacticle sensing fundamentals of piezoelectricity, New York, IEEE Press, 82.

Das, R., Choudhary, R.N.P., 2019. Studies of structural, dielectric relaxor and electrical characteristics of lead-free double Perovskite:Gd2NiMnO6. Solid State Sciences 87, 1-8.

David, G., 1999. Introduction to electrodynamics, 3rd edition, prentice hall, Inc, upper sandle river, New York, 37-46.

Erol, A., Ahmed, S., Ounaies, Z., von Lockette, P., 2019. A microstructure-based approach to modeling electrostriction that accounts for variability in spatial locations of domains. Journal of the Mechanics and Physics of Solids 124, 35-62.

Frederic, P.S., Christian, S., 2002. Mathematical structure of theoretical physics, DSA summer school, Gaesdonik, Germany, 27-34.

Gaikwad, A.S., Kadam, R.H., Shirsath, S.E., Wadgane, S.R., Shah, J., Kotnala, R.K., Kadam, A.B., 2019. Surprisingly high magneto-electric coupling in cubic Co0.7Fe2.3O4-SrTiO3 nano-composites. Journal of Alloys and Compounds 773, 564-570.

Gareeva, Z.V., Zvezdin, K.A., Pyatakov, A.P., Zvezdin, A.K., 2019. Novel type of spin cycloid in epitaxial bismuth ferrite films. Journal of Magnetism and Magnetic Materials 469, 593-597.

Herrera J.A., 2014. Piezoelectric technology influence by electromagnetic induction, New York, IEEE Press, 102.

Jin, L., Luo, W., Wang, L., Tian, Y., Hu, Q., Hou, L., Zhang, L., Lu, X., Du, H., Wei, X., Liu, G., Yan, Y., 2019. High thermal stability of electric field-induced strain in (1−x)(Bi0.5Na0.5)TiO3-xBa0.85Ca0.15Ti0.9Zr0.1O3 lead-free ferroelectrics. Journal of the European Ceramic Society 39, 277-286.

Jozef, H., Edwin, F.T., Slavormir, T., 2004. Deriving Lagranges equation using elementary calculus. American Journal of Physics 72(4), 510-513.

Kumar, D., Sarangi, S., 2019. Electro-magnetostriction under large deformation : Modeling with experimental validation. Mechanics of Materials 128, 1-10.

Kuzmina, J.S., Sytcher, G.A., Zaychenko, V.M., 2016. Performance evaluation of Absorber Reactors for solar fuel production. Chemical Engineering Transaction 61, 79-106.

Liu, P., Li, L., Wang, L., Huang, T., Yao, Y., Xu, W., 2019. Effects of 2D boron nitride (BN) nanoplates filler on the thermal, electrical, mechanical and dielectric properties of high temperature vulcanized silicone rubber for composite insulators. Journal of Alloys and Compounds 774, 396-404.

Ma, F., Clements, L.D., Hanna, M.A., 1998. Industrial and engineering, Chemistry Research 37, 3768-3771.

Michael, J., 2015. Simulation of time dependent schrodinger equation in the position of momentum domains, Chicago, USA, 24-37.

Sharma, S., Kumar, A., Gupta, V., Tomar, M., 2019. Dielectric and ferroelectric studies of KNN thin film grown by pulsed laser deposition technique. Vacuum 160, 233-237.

Xie, J., Yao, M., Gao, W., Su, Z., Yao, X., 2019. Significantly enhanced dielectric constant and energy density in Au/Al_2O_3 nanocomposite thin films. Journal of Alloys and Compounds 772, 324-331.

Xu, D., Yue, X., Zhang, Y., Song, J., Chen, X., Zhong, S., Ma, J., Ba, L., Zhang, L., Du, S., 2019. Enhanced dielectric properties and electrical responses of cobalt-doped $CaCu_3Ti_4O_{12}$ thin films. Journal of Alloys and Compounds 773, 853-859.

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