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

Chukwuemeka Peter Ukpaka

Department of Chemical/Petrochemical Engineering, Rivers State University Port Harcourt, Nigeria
*Corresponding author’s E. mail: chukwuemeka24@yahoo.com

INTRODUCTION

A dielectric is an electrical insulator that can be polarized by an applied 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
Research conducted on the insulator revealed that low electrical conduction and dielectric materials with a high polarizability possess the latter which is expressed by a number called the relative permittivity. The insulator is generally used to indicate electrical obstruction while the dielectric is used 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.

MATERIAL AND METHODS

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

\[
S_{ij} = Q_{ijkl} \times D_{l}
\]  

(1)
Where, \( S_{ij} \) is the strain components (unitless), \( D_i \) 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 various 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. 3:** Sample dielectric material with piezoelectric properties, showing the pooling direction and pressure (strain – Stress) (Clement et al., 1998).
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

---

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

**Fig. 5:** block diagram of the mathematical model.
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.

$$\frac{\varepsilon r}{\varepsilon_0} = \frac{C}{C_0} = \frac{\varepsilon}{\varepsilon_0}$$  

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.

$$P = \frac{p}{V}$$  

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.

$$p = ql$$  

Orientational polarization arises when there is a permanent dipole moment in the material. Materials such as HCl and H2O 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.

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

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).

$$\tau = pE \sin \theta$$  

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.

$$Ue = -pE \cos \theta = -P \cdot E$$  

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.

$$\kappa = 1 + \frac{\varepsilon e}{\varepsilon_0}$$  

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.

$$D = \varepsilon_0 E + P_{\text{total}}$$  

Where, E is the applied electric field, $\varepsilon_0$ is the vacuum permittivity and $P$ is the total polarization assuming the polarization is due to linear polarization.

$$P_{\text{total}} = P_{\text{linear}} = P_1$$  

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

$$R_1 = \varepsilon_1 \chi E$$  

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

$$\varepsilon_r = 1 + \chi$$  

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

$$D = \varepsilon_1 E + \varepsilon_1 \chi E$$  

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

$$D = \sigma = \frac{Q}{A}$$  

Piezoelectric polarization
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):

$$ S = s^E \cdot T + [d]^E \cdot E $$
$$ D = d^T + [g]^T \cdot E $$
$$ E = -g^T + [e]^T \cdot D $$

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.
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.

\[ \varepsilon = d \frac{E}{l} \]  

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

\[ \varepsilon = \frac{\Delta l}{l} \]

\[ \Delta l = d \frac{V}{l} \]  

\[ \Delta l = d \frac{l}{V} \]  

(Eq. 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 1×10⁶ Vm⁻¹, a corresponding polarization value of 0.5×10⁻⁴ cm². 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

fuel production. Chemical Engineering Transaction 61, 79-106.


Visit us at: http://bosaljournals.com/chemint/
Submissions are accepted at: editorci@bosaljournals.com