Model for the Creation of Electricity within a Piezoelectric Material under Strain

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Abstract-**This paper introduces the basis about piezoelectric effect. The reason why electricity is created in piezoelectric material under an external constrain is discussed in detail. The investigation is based on the basic structure of a molecule that composes piezoelectric crystals.**

Keywords – **Molecule, polarity, electrical potential, electrostatic field, electrostatic dipole, piezoelectricity.etc.**

I.INTRODUCTION

The term "Piezoelectricity" was used long time ago. It was the Curie brothers, Pierre and Jacques who brought it to light in Paris in 1880 [1]. This is a phenomenon found in some crystals under external excitation. An appearance of the charges occurs at the terminals of the crystals when a mechanical constrain is applied on it. Many practical applications have already been utilized since its discovery. In this paper, we will see the reasons for the appearance of charges in these crystals and the amount of charges that can be produced on one given structure. The study finds its basis from the bonding of atoms in the molecular structure.

II. MOLECULAR POLARITY

Molecules are built on atoms made of negatively charged electrons and positively charged nucleus. The distribution of these charges, positive and negative in a dipole, represents the polarity of a molecule. The latter is due to *(i)*the difference in electro negativity between the chemical elements that compose it, *(ii)*the differences in induced charges, and *(iii)*their distribution in space.

1. Electro negativity of Atoms and Bounds
The electro negativity of an atom [2] is a number that measures itsabilityto attract to itselfan electron pair involved in a chemical bond. Its value can be evaluated from the periodic table of elements. From the Pauling scale, it ranges from 4.0 (fluorine) to 0.7 (caesium and francium) [3].

The electro negativity difference between two atoms determines thetype of a bond: "pure" covalent bond (for two identical atoms), polar bond (covalent bond in which one of the two atoms is slightly more electronegative than the other one), nonpolar bond (the difference in electro negativity is small) Consider a bond between two atoms A and B. If atom B is slightly more electronegative than atom A, atom B will attract the electron pair rather more than atom A. The end of the bond at A will then become slightly positive with charge **δ+**, and the other end at B slightly negative with charge **δ-**.This results in a polar bond, that is a covalent bond in which there is a separation of charge between one end and the other.

2. Nonpolar Molecule
A molecule is nonpolar if the difference in electro negativity between the atoms is very small. So we have a uniform distribution of electrons. The "barycentre" of the charges **δ-** and that of the charges **δ+** coincide.

Silicon dioxide (SiO_2) is an example of a nonpolar molecule. It is formed of tetrahedral SiO_4 units bonded to each other by the oxygen atoms in a regular manner, as in quartz. Fig. 1 shows that the centroid of the molecule coincide with the middle of the silicon atom.
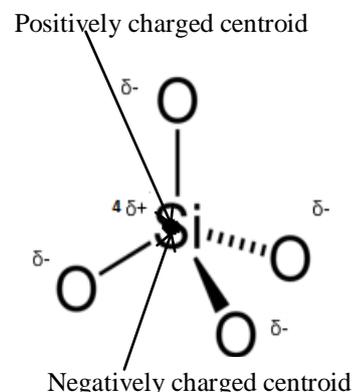

Fig.1 Molecular Structure of SiO_2.

3. Polar molecule

The molecule is polar if the electronegativity difference between atoms is greater than 0.4 [4]. The greater the difference between two atoms, the more electrons will be relocated to the most electronegative atom, and thus,the bond will be polarized. There is even an appearance of a positive partial charge and a negative partial charge which forms an instantaneous dipole or intrinsic polarization. Water which is symbolized by the formula $H_2O$is a polar molecule. The centre of the negative partial charges does not coincide with that of the positive partial charge, which is shown in Fig.2. The negative centre islocated in the oxygen atom and the positive center is in the middle of the two hydrogen atoms.
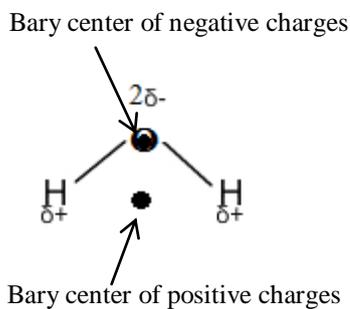
Bary center of negative charges

Bary center of positive charges

Fig. 2 Molecular Structure of H_2O.

III. PIEZOELECTRICITY PHENOMENON

An explanation in molecular scale can be given to the piezoelectric effect. This phenomenon is mainlydue to the spontaneous polarization of atoms in a molecule or in a crystal. Both types of molecule, polar and nonpolar can be piezoelectric.

If a crystal does not have intrinsic polarization (that is to say non polar), but the meshes of the lattice are such that the positive and/or negative ions are more abundant on one side than the other, then a compression can shift the barycentresof positive charges and negative charges. Theelectronic clouds of atoms move in relation to their natural position.

As it is a displacement compared to the electrically neutral situation, it appears as "mini-dipole". All these dipoles will create charges of the same sign on one side and opposite charges on the other side of the crystal [5]. These will create a global potential difference in the crystal. Figure 3 shows this phenomenon.

The crystals whose mesh has intrinsic or polar polarization can also have the phenomenon of piezoelectricity. The mechanism is analogous to those of crystals that have no intrinsic polarization.
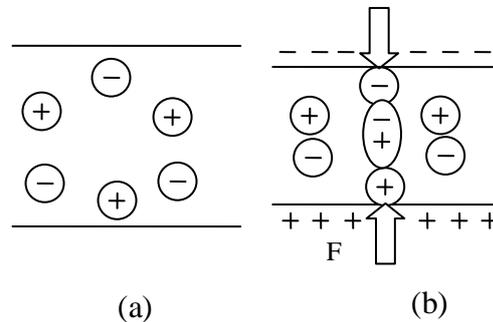

(a)   (b)

Fig.3(a) Molecule in the natural state, (b) Molecule under stress, appearance of opposite charges on both sides of the plate.

A compression or a mechanical expansion modifies the balance of the charges, which makes appear on the faces concerned a difference of potential. Figure 4 represents this case.
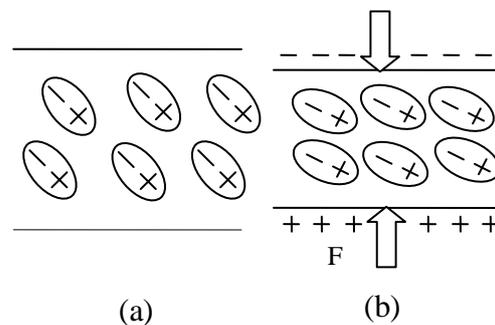

(a)   (b)

Fig.4(a) Molecule with intrinsic polarization in the natural state, (b) Molecule with intrinsic bias under stress, appearance of opposite charges on both sides of the plate.

In summary, the phenomenon of piezoelectricity is obtained by the creation or by the variation of an electrostatic dipole in the molecular structure of a crystal. The amount of charge obtained must be proportional to the sum of the potentials created by each electrostatic dipole in the crystal

IV. POTENTIAL AND FIELD CREATED BY A DIPOLE

An electrostatic dipole is defined by a set of distinct charges arranged in such a way that the centroid of the positive charges does not coincide with that of the negative charges. A simplest dipole consists of a set of two opposite point electric charges **+ q** and **- q**, separated by a distance awhich is very small compared to the distance **r**to the point **M** where their effects are to be observed [6].

1. Potential Created by a Dipole

Consider a dipole consisting of two opposite charges, **-q** and **+ q**, located respectively at a point A and B with $AB = a$.
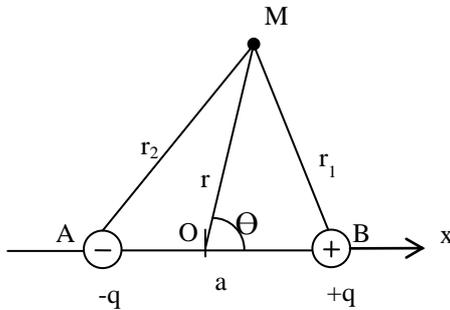

Fig.5 Presentation of a dipole with charge separation a.

One defines :
- **O** as the point in the middle of AB.
- **r** as the distance between O and M.
- $\mathbf{r_2}$ as the distance between A and M.
- $\mathbf{r_1}$ as the distance between B and M.
- **Ө** as the angle (Ox,OM).
- r >> a.

The potential V created at a point M by the dipole is:

$$V(M) = V_A(M) + V_B(M)$$
$$= \frac{1}{4\pi\varepsilon_0}\frac{-q}{AM} + \frac{1}{4\pi\varepsilon_0}\frac{+q}{BM}$$
$$= \frac{q}{4\pi\varepsilon_0}\left(\frac{1}{BM} - \frac{1}{AM}\right)$$

According to Pythagoras

$$BM^2 = (BO + OM)^2 = (OM + OB)^2$$
$$= OM^2 + OB^2 - 2OB.OM\cos\theta$$
$$= r^2 + \frac{a^2}{4} - ar\cos\theta$$

Let,

$$BM = r.\sqrt{1 - \frac{a}{r}\cos\theta + \frac{a^2}{4r^2}}$$

If Ө is replaced by $(\Theta - \pi)$,

$$AM = r.\sqrt{1 + \frac{a}{r}\cos\theta + \frac{a^2}{4r^2}}$$

From where

$$V = \frac{q}{4\pi\varepsilon_0 r}\left[\left(1 - \frac{a}{r}\cos\theta + \frac{a^2}{4r^2}\right)^{-\frac{1}{2}} - \left(1 + \frac{a}{r}\cos\theta + \frac{a^2}{4r^2}\right)^{-\frac{1}{2}}\right] \quad (1)$$

As $r >> a$, it means that $a/r << 1$

Using the development of $(1 + x)^n$ or $(1-x)^n$ limited to the first order, one obtains :

$$V = \frac{q}{4\pi\varepsilon_0 r}\left[\left(1 + \frac{a}{2r}\cos\theta\right) - \left(1 - \frac{a}{2r}\cos\theta\right)\right] \quad (2)$$

If $\vec{p} = q\overrightarrow{AB}$ is the dipole moment directed from **-q** to **+ q** and $\vec{e_r}$ the unit vector of $\overrightarrow{OM}$, then we have

$$V = \frac{q.a.\cos\Theta}{4\pi\varepsilon_0 r^2}$$
$$= \frac{\vec{p}.\vec{e_r}}{4\pi\varepsilon_0 r^2} \quad (3)$$

2. Dipolar Field

The field is calculated from the potential. We use the field-potential relationship:

$$E(M) = -\overrightarrow{grad}\,V(M)$$

Since V does not depend on Ө and **r**, only the components E_θ and E_r of $\vec{E}$ will be not zero. So we have:

$$\vec{E} = \begin{cases} E_r = -\dfrac{\partial V}{\partial r} = \dfrac{2p.\cos\Theta}{4\pi\varepsilon_0 r^3} \\[2mm] E_\theta = -\dfrac{1}{r}\dfrac{\partial V}{\partial\Theta} = \dfrac{p.\sin\Theta}{4\pi\varepsilon_0 r^3} \\[2mm] E_z = -\dfrac{\partial V}{\partial z} = 0 \end{cases} \quad (4)$$

The field created by a dipole is therefore proportional to $\frac{1}{r^3}$ and the potential to $\frac{1}{r^2}$, whereas for a point load, $\vec{E}$ which is created is proportional to $\frac{1}{r^2}$ and V to $\frac{1}{r}$.

For a distant point M, $\vec{E}$ and V that are created by a dipole will be negligible compared to $\vec{E}$ and V created by a nearby dipole.

To explain the origin of the basic equation of piezoelectricity, a simple uni dimensional representation is used.

V. EQUATIONS OF PIEZOELECTRICITY

Figure 6 shows an ionic structure between two atoms.

In the presence of an electric field $\vec{E}$, the negatively charged ions and the positively charged ions come

together in pairs. This movement displaces the electric centroids initially at the same position (when $E = 0$) and forms electric dipoles which naturally oppose the external disturbing field.
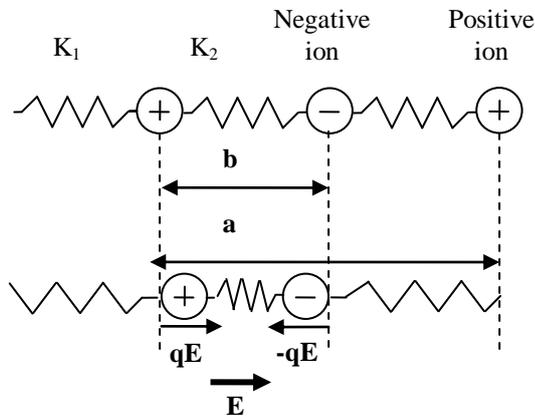

Fig.6 Deformation of a crystalline mesh of a piezoelectric material.

This ionic movement on the whole crystal subjected to the field produces a macroscopic deformation. This phenomenon is reversible since a mechanical contraction causes a similar displacement of the ions and the creation of dipoles (through the different stiffnessconstants K_1 and K_2). The appearance of an electric field occurs and then opposes the movement by electrostatic forces on the formed electric dipoles.

The charges **- q** and **+ q** are connected by springs which symbolizes the ionic bonds. The difference between K_1 and K_2 introduces the dissymmetry of the crystalmesh. An elementary cell of length **a** has two electric dipoles of moments$\frac{q}{2(a-b)}$and$\frac{-q}{2*b}$. Hence a dipole moment P_o:

$$P_0 = \frac{q}{2(a - 2b)} \qquad (5)$$

Then, the chain has the following properties:
- The polarization of the volumeisdifferent of zero if b is different from$\frac{a}{2}$.
- Under the effect of a constraint, the chain deforms the variation of the distances$a$ and$b$ cause a variation of the polarization (direct effect).
- Positive and negative ions moving in opposite directions under the action of an electric field and the ionic bonds not having the same stiffness, it results a deformation (converse effect).

The mechanical stresses T and strain$S$ are related to the electrical field$E$ and the induced polarization$P$ (or induction $D = \varepsilon_0 + P$).

The static equilibrium of each ion gives:

$$-qE + K_1\big(\Delta(a) - \Delta(b)\big) - K_2\Delta(b) = 0 \quad (6)$$

The force exerted by the right part of the chain on the left part is according to whether one is placed on the spring of stiffness K_1 or K_2:

$$F_1 = K_1\big(\Delta(a) - \Delta(b)\big)$$
$$F_2 = K_2\Delta(b)$$

A section S of the material has a large number of N chains per unit area. The mechanical tension T is therefore:

$$T = \frac{N}{2}K_1\big(\Delta(a) - \Delta(b)\big)$$
$$- \frac{N}{2}K_2\Delta(b) \qquad (7)$$

The induced polarization P is the polarization variation P_o with **n** density of the molecule $N = n*a$:

$$P = \Delta P_0 = \frac{nq}{2}K_1\big(\Delta(a) - 2\Delta(b)\big)$$
$$= -\frac{Nq}{2a}K_1\big(\Delta(a) - 2\Delta(b)\big)$$

By introducing the equilibrium relation (6), we obtain:

$$P = \Delta P_0 = \frac{qN}{2a}\left(\frac{2qE}{K_1 + K_2} + \frac{K_1 - K_2}{K_1 + K_2}\Delta(a)\right) \qquad (8)$$

P is the sum of two terms, the first proportional to the electric field E (dielectric effect) and the second proportional to the strain $S = \frac{\Delta(a)}{a}$ (piezoelectric effect). By plotting the expression of the polarization P as a function of the electrical displacement D, we find a typical equation for piezoelectricity:
$$D = \varepsilon E + eS \qquad (9)$$

From Equation (7), we deduce the second fundamental equation of piezoelectricity:
$$T = \varepsilon E - cS \qquad (10)$$

Piezoelectricity is generally transcribed in the form of these two equations, but under a tensor approach to the coupling between electrical and mechanical systems. It involves the electric displacement vectors D and the electric field E and the tensors of strain S and stress T:
$$\begin{cases} S = s^E T + d^t E \\ D = \varepsilon^T E + d\, T \end{cases} \qquad (11)$$

Concretely, these equations express the direct piezoelectricityeffect,it is the electric polarization of a ceramic subjected to a mechanical stress or the opposite effect by the deformation of a ceramic subjected to an electric field. These equations reflect well the linear

character of the piezoelectric effect and its dependence on the sign of the field and its amplitude. The choice of different input parameters makes it possible to define other characteristic equations [7]:

$$\begin{cases} T = C^D S - h^t D \\ E = \beta^s D - h\, S \end{cases} \tag{12}$$

$$\begin{cases} S = s^D T + g^t D \\ E = \beta^T D - g\, T \end{cases} \tag{13}$$

$$\begin{cases} T = c^E S - e^t E \\ D = \varepsilon^s E + e\, S \end{cases} \tag{14}$$

VI. CONCLUSION

The piezoelectric effect is a phenomenon that was discovered a long time ago. The phenomenon is generally based on the molecular structure of a crystal. Whatever the type of polar molecules whose centroid of the negative and positive partial charges does not coincide and has an instant dipole, or non polar with a bary center confused and has no intrinsic polarization, they may both be piezoelectric. A pressure subjected to a piezoelectric crystal causes a dissociation of the centroid of the positive and negative charges in the case of the nonpolar molecules, mini dipoles will be created and which will cause a potential difference across the crystal (which gives electricity). In the case of the polar molecule, the pressure will reorient the intrinsic dipoles in the opposite direction. This will give the difference of potential at the terminals.

One-dimensional modeling was done to explain the properties of piezoelectric materials. The ionic bond between positive and negative ion is replaced by a spring of stiffness K. The study shows that the polarization P which is a function of the electric displacement D can be represented by the sum of two terms E (dielectric effect) and S (deformation).

$$D = \varepsilon E + eS$$

And the mechanical stress T can be presented by:

$$T = \varepsilon E - cS$$

The other basic equations for piezoelectricity can then be deduced. They are presented in equation (11), (12), (13) and (14).

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