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Using Smart-Piezoelectric Materials to Generate Electricity

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Abstract

This research represents the theoretical study introduction to generate electricity by using the smart piezoelectric materials to design a smart system, that transforms the mechanical stresses into electrical output or pulses, for obtaining sufficient and clean electrical energy, and use it to offset some of the power coming from the main grid. Because of the constant demand for energy, high costs, and the depletion of natural resources, we must provide secondary solutions of energy production, in line with the environment and economy. So we are study generating electricity by piezoelectric materials, from easy sources such as walking, sounds, pressure or traffic, for running street lighting, a billboard, or otherwise. Another objective of research, is employing the smart materials to design a smart system, and experience it in engineering application in Libya.

Keywords: Smart Materials, Piezoelectric Materials, Generation Energy, Energy Harvesting.

1. Introduction

1.1 Historical Background

This term "**Piezoelectricity**" used to describe the ability of certain materials to develop an electric charge that is directly proportional to an applied mechanical stress, and these also showing the converse effect. And This term has involved two sections: first section (**Piezo**), is from the Greek word "**piezein**", which means "**to press tightly or squeeze**", and second section (**Electricity**). The uniform meaning is "**squeeze electricity**" (Bohidar, et al., 2015) (Dictionary, 2019).

The Piezoelectric effect was initially observed by the French physicists *Jacques & Pierre Curie* in 1880, they discovered a connection between the macroscopic piezoelectric phenomena and the Crystallographic structure in crystals of sugar, quartz and Rochelle salt, where that an electrical output was produced when imposed a mechanical strain on those materials. They demonstrated this coupling by measuring the charge induced across electrodes placed on the material, when it underwent an imposed deformation. The converse effect was first mathematically deduced from fundamental thermodynamic principles by *Lippmann* in 1881, later the *Curie* brothers demonstrated it. The property was interesting, but The electromechanical coupling is not very useful, because the amount of electrical signal was "small" and not exist precise instrumentation for measuring output (Leo, 2007) (Varadan, et al., 2006).

Due to World War I, interest in piezoelectricity increased. In 1917 *Paul Langevin* developed an underwater device, a transducer that utilized a piezoelectric crystal to produce a mechanical signal and measure its electrical response as a means of locating submarines, this work was the basis of Sonar and became one of the first engineering applications for the piezoelectricity. And World War II stimulated even more advance in the piezoelectric materials and devices, *Frederick Lack* developed a crystal that operated through a wide range of temperatures, this development allowed the use of aviation radio and engage mass attacks. In Japan, a temperature stable crystal was developed by *Issac Koga*, major developments included new designs of ceramic filters. In addition to improvements in sonar, developments in electronics began as electronic oscillators, filters, buzzers, and audio transducers (Leo, 2007) (Varadan, et al., 2006).

Barium-Titanate ($BaTiO_3$) was an early synthetic piezoelectric material that had piezoelectric and thermal properties that made it superior to quartz crystals, and the polymeric materials such as **Poly vinylidene fluoride (PVDF)**, have also been shown to exhibit similar characteristics. Intense research is still going on to produce useful and reasonably priced actuators, which are low in power consumption and high in reliability and environmental ruggedness (Varadan, et al., 2006).

1.2 Definitions and Clarifications

1.2.1. Smart Materials

Are those materials that exhibit coupling between multiple physical domains. By other words; are those that convert energy between multiple physical domains. Common examples of these materials include those that can convert electrical signals into mechanical deformation and can convert mechanical deformation into an electrical output, and the materials that convert thermal energy to mechanical strain, and even those that couple the motion of chemical species within the material to mechanical output or electrical signals. Other names for these types of materials are intelligent materials, adaptive materials, and even structronic materials (Leo, 2007). Smart materials are usually attached or embedded into the structural systems to enable these structures to sense disturbances, process the information and evoke reaction at the actuators, Thus, smart materials, respond to environmental stimuli and for that reason are also called responsive materials (Varadan, et al., 2006).

1.2.2. Smart System Structure

Smart materials system is the engineering system that utilizes the coupling properties of smart materials to provide functionality (Leo, 2007). And should respond to internal (intrinsic) and environmental (extrinsic) stimuli. To do this, they should have sensors and actuators embedded in them:

● **Transducer:** A device that is actuated by power from one system and supplies power, usually in another form, to a second system.
● **Sensor:** A device that responds to a physical stimulus as heat, light, sound, pressure, magnetism or a particular motion, and transmits a resulting impulse, as for measurement or operating a control.
● **Actuator:** One that actuates, e.g. a mechanical device for moving or controlling something (Varadan, et al., 2006).

As described earlier, the smart structure is a system that incorporates particular functions of sensing and actuation to perform smart actions in an ingenious way, and it is need sensors, actuators and a controller, as shown in (**Figure 1**) (Varadan, et al., 2006).

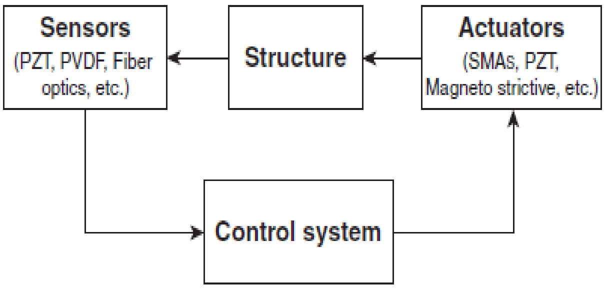

Figure 1 Building blocks of a typical smart system.

In addition to having sensing and/or actuation properties, smart materials have to fulfill the requirements and the further favorable characteristics as follows:

● **Technical properties** (e.g. Mechanical, behavioral, thermal, electrical).
● **Technological properties** (e.g. Manufacturing, forming, welding abilities, thermal processing, waste level, workability).
● **Economic aspects** (e.g. Raw material and production costs, supply, availability).
● **Environmental characteristics** (e.g. Toxicity, pollution, possibility of reuse or recycling) (Akhras, 2000).

The basic five components of a smart structure are summarized as follows, and are shown in (**Figure 2**):

● ***Data Acquisition (tactile sensing):*** the aim of this component is to collect the required raw data needed for an appropriate sensing and monitoring of the structure.
● ***Data Transmission (sensory nerves):*** the purpose of this part is to forward the raw data to the local and/or central command and control units.
● ***Command and Control Unit (brain):*** the role of this unit is to manage and control the whole system by analyzing the data, reaching the appropriate conclusion, and determining the actions required.
● ***Data Instructions (motor nerves):*** the function of this part is to transmit the decisions and the associated instructions back to the members of the structure.
● ***Action Devices (muscles):*** the purpose of this part is to take action by triggering the controlling devices/units (Akhras, 2000).

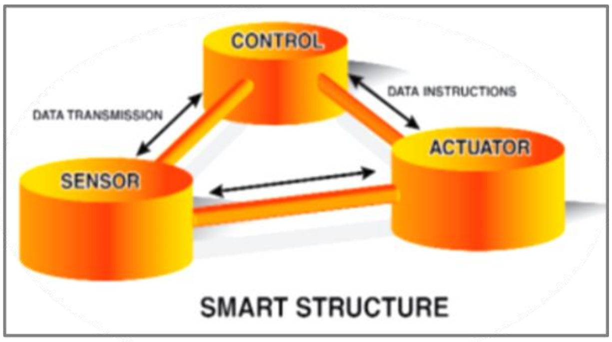

Figure 2 The Basic Five Components of a Smart Structure.

1.2.3. Piezoelectric Materials

Are those materials that convert energy between the mechanical and electrical domains (Leo, 2007). The application of the electrical field causes the material to expand or contract almost instantly, the converse effect has also been observed (Varadan, et al., 2006).

● ***The direct effect*** when a material subjected to a mechanical stress becomes electrically charged. Thus, these devices can be used to detect strain, movement, force, pressure, or vibration by developing appropriate electrical responses.

● ***The converse effect*** when placed the material in an electric field, it becomes strained. This ability can be used to generate a movement, force, pressure, or vibration by applying a suitable electric field (Schwartz, 2002).

These materials have already found several uses in actuators, which has led to their use as sensors (Varadan, et al., 2006).

Piezoelectric materials have wide applications ranging from everyday use to more specialized devices (**Table 1**) (Elkhider, 2015).

Table 1 Some application areas of piezoelectric materials.

Industry	Application
Automotive	Air bag sensor, air flow sensor, audible alarm, fuel atomizer, keyless door entry, seat belt buzzer, knock sensor.
Computer	Disc drives, inkjet printers.
Consumer	Cigarette lighters, depth finders, fish finders, humidifiers, jewelry cleaners, musical instruments, speakers, telephones.
Medical	Disposable patient monitors, fetal heart monitors, ultrasonic imaging.
Military	Depth sounders, guidance systems, hydrophones, sonar.

And (**Figure 3**) shows the market forecast for piezoelectric transducers by region up to 2022 (Elkhider, 2015).

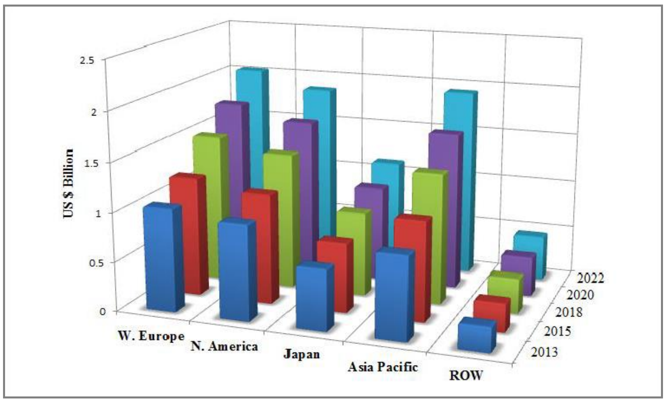

Figure 3 The market forecast for piezoelectric transducers.

1.2.4. Physical Domains & Types Coupling

The domain is any physical quantity that we can describe by a set of two state variables. An example of the physical domain is the mechanical domain, whose state variables are the states of stress and strain within a material. Another example is the electrical domain, whose state variables are the electric field and electric displacement of a material. Other examples are of domains in (**Figure 4**) (Leo, 2007).

Mechanical	Electrical	Thermal	Magnetic	Chemical
Stress	Electric field	Temperature	Magnetic field	Concentration
Strain	Electric displacement	Entropy	Magnetic flux	Volumetric flux

Figure 4 Physical domains and associated state variables.

The Coupling occurs when a change in the state variable in one physical domain causes a change in the state variable of a separate physical domain. For example, changing the temperature of a material, which is a state variable in the thermal domain, can cause a change in the state of strain, which is a mechanical state variable. And the mentioned example is called the Thermo-mechanical coupling, where the coupling is denoted by a term that is a combination of the names associated with the two physical domains.

A visual representation of the notion of physical domains and the coupling between them is shown in (**Figure 5**). Each rectangle represents a single physical domain. Listed in each rectangle are the state variables associated with the domain. The bridge within the rectangle is the physical property that relates to the state variables. The elastic properties of a material relate the states of stress and strain in the material, and the dielectric properties relate the electrical state variables. Coupling between the physical domains is represented by the arrows that connect the rectangles (Leo, 2007).

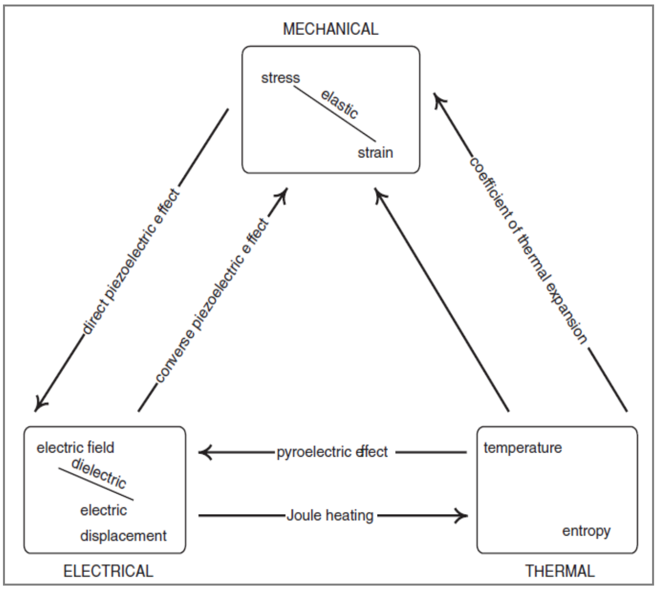

Figure 5 The coupling between the physical domains.

1.2.5. Classification Of Smart Materials

Examples of smart materials are shown in (**Table 2**) (Varadan, et al., 2006), and can be grouped into the following categories:

● **Thermoresponsive materials:** Shape memory alloys (SMAs) are another widely used type of smart materials, which change shape in response to changes in temperature. Once fabricated into a specified shape, these materials can retain/regain their shape at certain operating temperatures. They are therefore useful in thermostats and in parts of automotive and air vehicles. The most common commercially available shape memory alloy is National. This alloy is very ductile and can be deformed easily. In addition, it also has good strength and strain rate, it is corrosion resistant, and it is stable at high temperature (Varadan, et al., 2006) (Schwartz, 2002).

● **Electrostrictive materials:** These materials can also change their dimensions significantly on the application of an electric field; the effect is reciprocal as well. Although the changes thus obtained are not linear in either direction, these materials have also found widespread application in medical and engineering fields. The most popular electrostrictive material is lead magnesium niobate (PMN), (Varadan, et al., 2006) (Schwartz, 2002).

● **Optical fibers:** Optical fibers make excellent strain sensors because they are immune to electromagnetic interference. The more useful fiber-optic strain sensors uses the intrinsic properties of the optical fiber. In an intrinsic fiber measurement, one or more of the optical field parameters, which include frequency, wavelength, phase, mode index, polarization, index of refraction, and attenuation coefficient, are affected by the environment (Schwartz, 2002).

● **Rheological materials:** While the materials described above are all solids, rheological materials are in the liquid phase. These can change state instantly through the application of an electric or magnetic charge. These fluids may find applications in brakes, shock absorbers and dampers for vehicle seats (Varadan, et al., 2006).

● **Electrochromic materials:** is the ability of a material to change its optical properties (e.g. Color) when a voltage is applied across it. These are used as antistatic layers, electro-chrome layers in liquid crystal displays (LCDs) and cathodes in lithium batteries (Varadan, et al., 2006).

● **Smart gels:** These are gels that can shrink or swell by several orders of magnitude (even by a factor of 1000). Some of these can also be programed to absorb or release fluids in response to a chemical or physical stimulus. These gels are used in areas such as food, drug delivery and chemical processing (Varadan, et al., 2006).

Table 2 Examples of materials used in smart systems.

Development stage	Material type	Examples
Widely commercialized	Shape memory alloys	NITINOL
	Piezoelectric	PZT-5A, 5H
	Electrostrictive	PMN-PT
Early commercialization or under development	Magnetostrictive	Terfenol-D
	Fiber-optic sensor	---
	Conductive polymers	
	Chromogenic	
	Electrorheological Magnetorheological	
Early research and development	Biomimetic polymers & gels	
	Fullerenes & carbon nanotubes	

A brief comparison of some of the electromechanical transducers is presented in (**Table 3**) (Varadan, et al., 2006).

Table 3 Comparison of electromechanical transducers.

Actuator	Fractional stroke (%)	Max. energy density (J/cm^3)	Efficiency	Speed
Electro-static	32	0.004	High	Fast
Electro-magnetic	50	0.025	Low	Fast
Piezo-electric	0.2	0.035	High	Very fast
Magneto-strictive	0.2	0.07	Low	Very fast
Electro-strictive	4	0.032	High	Fast
Thermal	50	25.5	Low	Slow

Where the actuators based on piezoelectricity, magnetostriction and electrostriction depend on changes in strain produced by an applied electric or magnetic field in materials used. Both electrostrictive and piezoelectric materials deform with the application of an electric field, but while the relationship between the force produced and applied field is linear in piezoelectrics, it is quadratic in electrostrictive materials (Varadan, et al., 2006).

The general characteristics of commercially available actuators are shown in (**Table 4**). Typically, can be evaluated the performance of an actuator in terms of the characteristics, e.g. Displacement (**the ability of the actuator to displace an object**). Force generation (**the amount of force the actuator can produce**). Hysteresis (**the degree of reproducibility in positioning operations**). Response time (**how quickly an actuator can start the actuation process**). Bandwidth (**the range of frequencies in which the actuator can operate effectively**). Temperature range of operation, Power required to drive the actuator, Repeatibility, Precision, Mass required, and Cost (Schwartz, 2002) (Akhras, 2015).

Table 4 Actuator technology assessment.

	Nitinol	Terfenol-D	PZT
Energy	Heat	Magnetic field	Electric field
Hysteresis	High	Low	Low
Bandwidth	Low	Moderate	High
Accuracy	Poor	High	High
Response time	Low	Fast	Very fast
Power use	High	Moderate	Moderate
Maturity	New	New	Established
Strain capacity	3000 - 5000 μ	1300 - 2000 μ	600 - 1000 μ

The piezoelectric PZT provides the potential for the greatest force handling capability, and also operates across the highest bandwidth of the micro-actuators and has among the highest displacements. Piezoelectrics have higher bandwidths than are possible in shape memory alloys (Nitinol), they are more compact than magnetostrictive devices, and they are bidirectional by nature, unlike electrostrictive materials (Schwartz, 2002).

And can be evaluated The performance of any sensor in terms of Sensitivity (**amount of signal that a sensor produces for a given change in the variable**), The length across which the measurement is made, Bandwidth (**the frequency range over which the sensor remains effective**), Response time (**the speed at which the sensor can respond to a change in the variable**), Temperature range of operation, Repeatability, Precision and Cost. Relative assessment of the sensor types considered suitable for embedding in adaptive composite systems in (**Table 5**) (Schwartz, 2002).

Table 5 Sensor technology assessment.

	Fiber Optics	**PZT**
Sensitivity	Moderate	Moderate
Gauge length	Moderate	High
Bandwidth	High	Moderate
Resolution	High	Moderate
Temperature range	High	High

Piezoelectric sensors tend to operate best in dynamic situations because the induced charge imbalances created by straining the material dissipate with time, How quickly this occurs depends on the material's capacitance, resistivity, and output loading (Schwartz, 2002).

1.3 Physical mechanisms

Piezoelectricity linearly relates an induced polarization to an applied stress, by other word, is linear interaction between mechanical and electrical systems in non-centric crystals or similar structures, as shown in (1)

$$P_i = d_{ijk}\sigma_{jk} \qquad (1)$$

Where $\boldsymbol{\sigma}_{jk}$ is the applied stress, $\boldsymbol{P}_i$ is the induced polarization, and $\boldsymbol{d}_{ijk}$ is the piezoelectric charge coefficient.
The direct piezoelectric effect is the change of electric polarization proportional to the strain. A material is said to be piezoelectric if the application of an external mechanical stress gives rise to dielectric displacement in this material. This displacement manifests itself as internal electric polarization. It should be noted that the piezoelectric effect strongly depends on the symmetry of the crystal. A crystal having sufficiently low symmetry produces electric polarization under the influence of external mechanical force. Crystals belonging to the 11 point groups having central symmetry are unable to produce piezoelectric effect. With one exception, all classes devoid of a centre of symmetry are piezoelectric. The single exception is the Class 29 (enantiomorphous hemihedral), which, although without a centre of symmetry, nevertheless has other symmetry elements that combine to exclude the piezoelectric property. Closely related is the converse effect, whereby a piezoelectric crystal becomes strained if an external electric field is applied. Both effects are the manifestation of the same fundamental property of the non-centric crystal (Tichý, et al., 2010).

As shown in (**Figure 6**) of the 32 crystallographic point groups, only 21 are noncentrosymmetric. The piezoelectricity a null property in centrosymmetric structures. In the same way, in point group 432, the combination of symmetry elements eliminates piezoelectricity. The remaining 20 point groups are potentially piezoelectric. Of these 20 point groups, ten are polar, that is, they have a vector direction in the material that is not symmetry-related to other directions. Such materials can have a spontaneous polarization, which is typically a function of temperature. Thus, these materials are pyroelectric. Ferroelectric materials are a subset of pyroelectric materials in which the spontaneous polarization can be reoriented between crystallographically-defined directions by a realizable electric field. Thus, all ferroelectric materials are both piezoelectric and pyroelectric. While symmetry considerations can describe whether a material is potentially piezoelectric, they provide no information on the magnitude of the piezoelectric response (Safari & Akdogan, 2008).

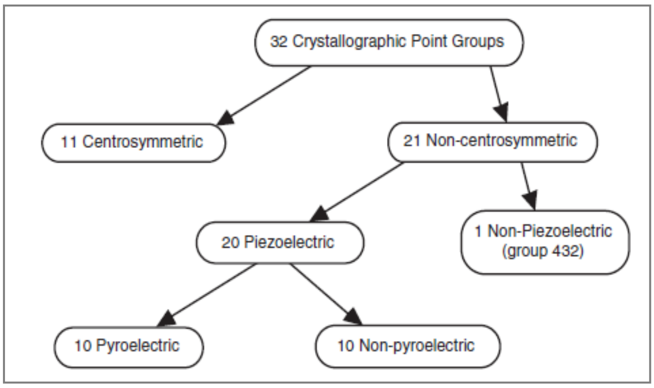

Figure 6 Symmetry hierarchy for piezoelectricity.

1.4 Piezoelectric Materials

Piezoelectric materials is ceramics or polymers which can produce a linear change of shape in response to an applied electric field (Varadan, et al., 2006). Some certain ceramics and crystals commonly used as piezoelectric materials are solid materials show good piezoelectric property, it used in various applications such as medical, aerospace, consumer electronics, and even automotive industry. But cannot be used in biomedical applications due to its rigid, and high acoustic impedance characteristics of piezoelectric crystals.

However, previous studies found that such as polymers like Poly vinyl carbonate (**PVC**), Nylon 11, and polyvinylidene fluoride (**PVDF**) also show piezoelectricity. **PVDF** polymer is lightweight, flexible, and has low acoustic impedance and high piezoelectric constant therefore, is a good candidate for sensors because of its piezoelectric voltage constant around (216 $\frac{V/m}{N\,/\,m^2}$). **PVDF**'s piezoelectric voltage constant is about 20 times higher than PZT (6.6 $\frac{V/m}{N\,/\,m^2}$). And 40 times higher than Barium titanate (10 $\frac{V/m}{N\,/\,m^2}$). PVDF polymer shows much lower density and acoustic impedance than piezoelectric crystals, which enables its usage for biomedical or acoustic sensing (Kim, 2015).

Polyvinylidene fluoride (**PVDF**) is a fluorinated thermoplastic polymer with low density compared to other fluoropolymers. Due to its polar crystalline structure, PVDF has excellent piezoelectric properties by itself, compared to other polymeric materials. PVDF consists of at least five different structural forms depending on whether the chain is in ***trans*** (**T**) or ***gauche*** (**G**) linkage. The most common PVDF varieties are identified as (**α-non-polar**) or (**β-polar**) form. Although the (**α-phase**) exists in large quantities compared to the (**β-phase**), it is the later (**β-phase**) that is responsible for the piezoelectric response of PVDF. (**Figure 7**) shows the (**β-phase**) has a higher degree of polarity with oriented hydrogen and fluoride (**CH_2–CF_2**) unit cells along the carbon backbone. In order to obtain (**β-PVDF**), electrical poling and mechanical stretching processes are required during the manufacturing process to align the dipoles in the crystalline PVDF structures. (Elkhider, 2015).

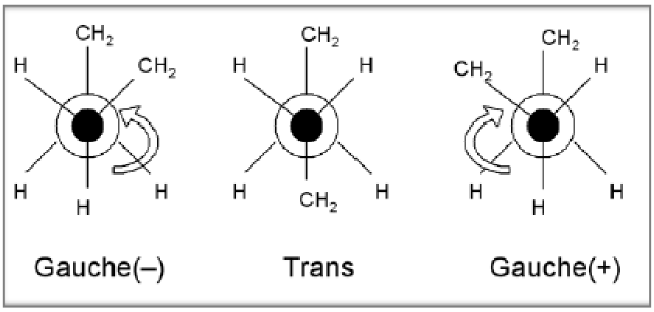

Figure 7 (a) Newman projections conformations of the bonds around each carbon atom.

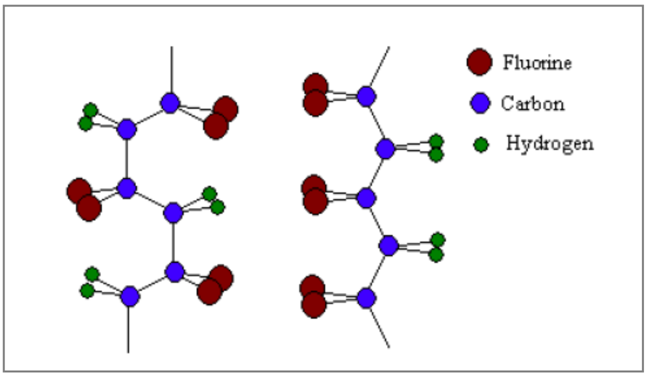

Figure 7 (b) Crystal structure of PVDF: Non-polar α-phase (L), and polar β-phase (R).

■ **Polymeric Materials:**

1) **PVDF (polyvinylidene fluoride)**
2) **PVF (polyvinyl fluoride)**
3) **PTFE (poly tetrafloroethylene)**
4) **PTFE (poly trifluoroethylene)**
5) **PVDC (polyvinylidene carbonate)**
6) **PVC (polyvinyl carbonate)**
7) **(polyvinyl chloride)**
8) **Nylon 11**

(Elkhider, 2015) (Kim, 2015).

■ **Ceramic Materials:**

1) **Lead zirconate titanate (PZT)**
2) **Lead titanate ($PbTiO_3$)**
3) **barium titanate ($BaTiO_3$)**
4) **Bismuth titanate ($Bi_4Ti_3O_{12}$)**
5) **Lead magnesium niobate (PMN)**
6) **Lithium niobate ($LiNbO_3$)**
7) **Lithium tantalate ($LiTaO_3$)**
8) **Lithium tetraborate ($Li_2B_4O_7$)**
9) **Potassium niobate ($KNbO_3$)**
10) **Zinc oxide (ZnO)**
11) **Gallium Orthophosphate ($GaPO_4$)**

(Tichý, et al., 2010) (Sharapov, 2011).

Some Properties of piezoelectric materials in (**Table 6**) (Fraden, 2016).

Table 6 Properties of piezoelectric materials at 20° C.

	Symbol	**PVDF**	**$BaTiO_3$**	**PZT**
Density	**(*10^3 kg/m^3)**	**1.78**	**5.7**	**7.5**
Piezo-electric constant	**(pC/N)**	**d_{31}= 20** **d_{32}= 2** **d_{33}= -30**	**78**	**110**
Electro-mechanical coupling constant	**(%)**	**11**	**21**	**30**
Acoustic impedance	**(10^6 kg/m^{2}s)**	**2.3**	**25**	**25**

1.5 Applications of Piezoelectricity

■ **The summery of energy harvesting techniques studies:**

Mechanical sources provide a promising alternative to harvest energy where vibration source is the best. Vibrations in some situations can be very large, like in case of the vibrations of civil structures like tall buildings, railroads, ocean waves, & even human motions & can give a better output power. Sources for conversion of vibration energy into electrical energy include electrostatic, magnetic field, or strain on a piezoelectric material (Sil, et al., 2017).

● A study has been done on energy harvester mounted on sneakers that generated electrical energy from pressure on the shoe sole. The first energy harvesters had multilayer laminates of PVDF, the second one contained a PZT unimorph & the third one was a rotary electromagnetic generator. Another study described that the high temperature energy harvester, incorporating silicon carbide electronics & a PZT energy harvester can operate at 300 Celsius. A mini-scale electromagnetic energy harvester prototype that consists of a coil & a silicon wafer cantilever beam with four pole magnets, shown in (**Figure 8**) (Sil, et al., 2017).

● The vibrations energy harvesting principle using piezoelectric materials into designing piezoelectric generator & installed it on a bicycle handlebar to supply portable electrical energy was done, this experiments that have conducted have shown that the few mW that produced by the piezoelectric generator is able to power bike LED lamp. A static converter transforms the electrical energy in a suitable form to the targeted portable application.

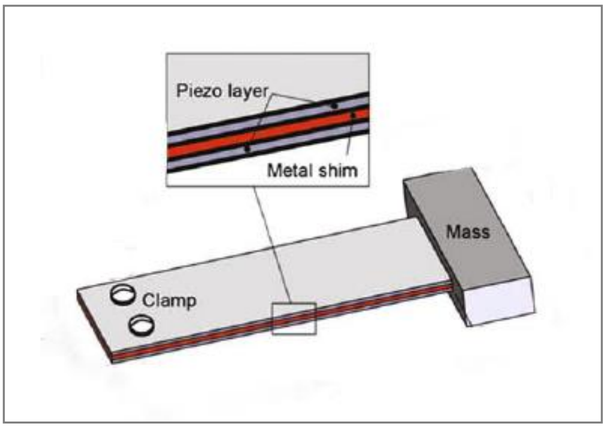

Figure 8 PZT coated cantilever beam.

● Another study proposes circuit of an energy harvesting, it which consists of an AC–DC rectifier with an output capacitor, an electrochemical battery, & a switch-mode DC–DC converter that controls the energy flow into the battery. A PZT model for harvesting energy from structural sensors on a bridge or global positioning service (GPS) tracking devices was developed. Where the researchers establishing an experimental method to calculate charge accumulated on the surface of the PZT layer under applied strain. This model in turn simplifies design procedure necessary for determining the appropriate size & vibration levels which is necessary for accurate sufficient energy to be produced & supplied to the electronic devices (Sil, et al., 2017).

■ **Various other applications:**

Piezoelectricity links the fields of electricity and acoustics. Consequently, Piezoelectric materials are key components in acoustic transducers such as microphones, loudspeakers, transmitters, burglar alarms and submarine detectors (Stein & Powers, 2006). The various applications can be summarized as follows:

● First engineering application for the piezoelectricity, is present day sonar systems, by using quartz crystals in an ultrasonic sending and detection system (Leo, 2007).

● One such idea that will fit well in an airport setting is the capturing of kinetic energy from passenger foot traffic, this novel idea is not only clean, but it is also renewable, the use of piezoelectric devices installed in airport terminals will enable the capturing of kinetic energy from foot traffic.

● They can also be used in optical-tracking devices, magnetic heads, dot-matrix printers, computer keyboards, high-frequency stereo speakers, accelerometers, micro-phones, pressure sensors, transducers, and igniters for gas grills (Kamila, 2013).

● Another simple application by creating shoe that can generate electricity, by attached the transducers to an insole of a shoe, and then are connected to a rectifier to convert the AC into a DC (Sil, et al., 2017).

(**Figure 9**) gives a summarized outline of technical applications of piezoelectricity (Tichý, et al., 2010).

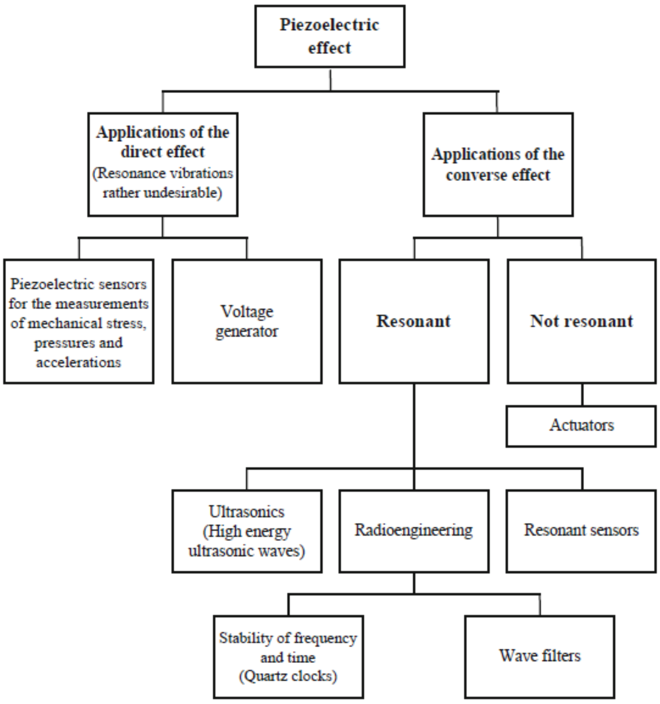

Figure 9 Technical applications of piezoelectricity.

2. Calculation

2.1 Calculation of Polarization

We can quantify the nature of polarization (Shackelford, 2015), for example in $BaTiO_3$ by use of the concept of a dipole moment, which is defined as the product of charge $\boldsymbol{Q}$, and separation distance $\boldsymbol{d}$. Calculate the total dipole moment for (**a**) the tetragonal $BaTiO_3$ unit cell and, (**b**) the cubic $BaTiO_3$ unit cell.

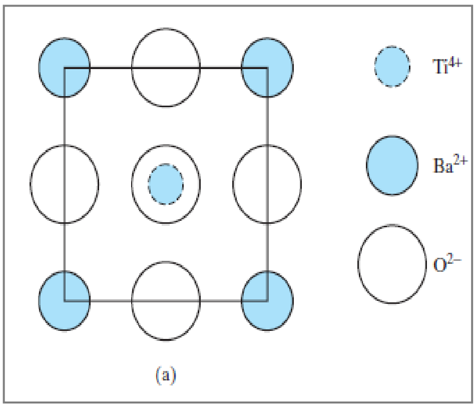

Figure 10 (a) Front view of the cubic $BaTiO_3$ structure.

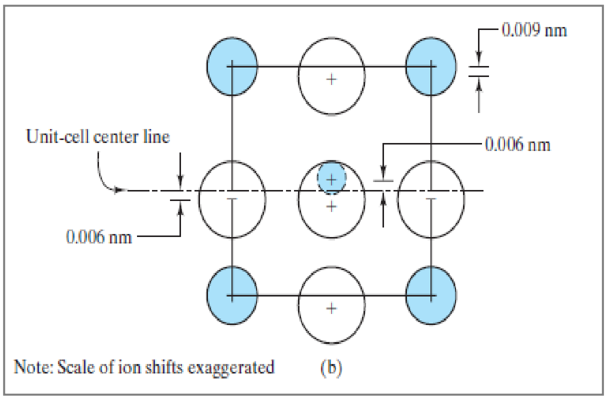

Figure 10 (b) Below 120° C, a tetragonal modification of the structure occurs. The net result is an upward shift of cations and a downward shift of anions.

(a) Using **Figure 10 (b)**, we can calculate the sum of all dipole moments relative to the midplane of the unit cell (indicated by the center line in the figure). A straightforward way of calculating the ***Qd*** would be to calculate the ***Qd*** product for each ion or fraction thereof relative to the midplane and sum. However, we can simplify matters by noting that the nature of such a summation will be to have a net value associated with the relative ion shifts. For instance, the Ba^{2+} ions need not be considered because they are symmetrically located within the unit cell. The Ti^{4+} ion is shifted upward 0.006 nm, giving

Ti^{4+} moment = (+4q) (+0.006 nm).

The value of ***q*** as the unit charge **(= 0.16 * 10^{-18} C)**, giving

Ti^{4+} moment = (1 ion)(+4 * 0.16 * 10^{-18} C/ion)
(+6 * 10^{-3} nm)(10^{-9} m/nm)
= +3.84 * 10^{-30} C * m.

Inspection of the perovskite unit helps us visualize that two-thirds of the O^{2-} ions in $BaTiO_3$ are associated with the midplane positions, giving (for a downward shift of 0.006 nm)
O^{2-} (midplane) moment = (2 ions)(-2 * 0.16 * 10^{-18} C/ion)
(-6 * 10^{-3} nm)(10^{-9} m/nm)
= +3.84 * 10^{-30} C * m.

The remaining O^{2-} ion is associated with a basal face position that is shifted downward by 0.009 nm, giving

O^{2-} (base) moment = (1 ion)(-2 * 0.16 * 10^{-18} C/ion)
(-9 * 10^{-3} nm)(10^{-9} m/nm)
= +2.88 * 10^{-30} C * m.

Therefore,

∑Qd = (3.84 + 3.84 + 2.88) * 10^{-30} C * m
= 10.56 * 10^{-30} C * m.

(b) For cubic $BaTiO_3$ [**Figure 10(a)**], there are no net shifts and, by definition,

∑Qd = 0.

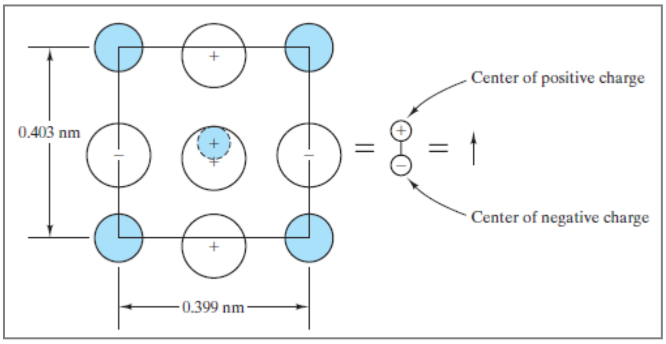

Figure 11 The tetragonal unit cell shown in **Figure 10 (b)** is equivalent to an electrical dipole (with magnitude equal to charge times distance of separation).

Using the results of last example, and the unit cell geometry of (**Figure 11**), we obtain

$$P = \frac{\sum Qd}{V}$$

$$\frac{10.56 * 10^{-30}(C * m)}{(0.403 * 10^{-9}m)(0.399 * 10^{-9}m)^{2}}$$

= 0.165 C/m^2

3. Conclusions

1) Piezoelectric energy harvesting is a very interesting concept, in present day life, where there is a great demand for energy.
2) It is best suitable and also very efficient way of energy harvesting. Piezo - Smart Materials convert the mechanical stress applied on it, into electrical energy.
3) This electrical energy is further stored in a device like lithium polymer batteries so that it can be used in portable devices such as mobile phones or other hand held electrical devices.
4) Using Piezo - Smart Materials are very reliable as it uses the movement of man such as walking, jogging etc, to produce energy. The rectifier, DC–DC

converter and battery charging circuit used in the project contains minimum number of components and hence it is very compact.

5) Low cost and the future changes can be made without much difficulty in the hardware. The inclusion of further components in the circuit can be made easily.

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