International Journal of Science and Research (IJSR)
ISSN: 2319-7064
SJIF (2022): 7.942

Optimizing Piezoelectric Nanogenerators for Efficient Wearable Health Monitoring Systems

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Abstract: ***This study investigates the simulation - based optimization of piezoelectric nanogenerators (PENGs) for autonomous health monitoring sensors. PENG enables the continuous and independent functioning of health monitoring equipment by converting mechanical energy from body motions into electrical energy. This work optimizes the energy harvesting efficiency of $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (x = 0.1 and y = 0.05) based PENG by using density functional theory. Numerous elements are included in the analysis, such as doping impact and piezoelectric material choices. This study enables to determine the high d_{33} value = 830 pC/N and output voltage 18 V for $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (x = 0.1 and y = 0.05) based PENG. The enhanced PENG is suitable for wearable health monitoring applications, as evidenced by the results, which show a considerable change in the piezoelectric constant d_{33}. By improving the quality of piezoelectric material, this research helps to design novel health monitoring systems.***

Keywords: Nanomaterials, Nanogenerators, Piezoelectric Nanogenerator (PENG), Self - Powered Sensors**,** Piezoelectric Materials**,** First Principle Theory, Density Functional Theory

1. Introduction

The continual need for more sophisticated health monitoring systems has lead research toward self - powered sensors that can track physiological variables continuously without the need for external power sources [1]. Efficiency and long - lasting power solutions are the basic needs, as evidenced by the latest advancements in wearable and implantable health monitoring systems [2, 3]. Long - term use and patient comfort are hampered due to the short lifespan and frequent charging or replacement of traditional batteries, which power these devices. In an effort to overcome these obstacles, scientists are investigating systems known as energy - harvesting, which harvest energy from human - generated or ambient sources such as vibrations, motion, and temperature changes. Out of all the energy - harvesting methods, piezoelectric nanogenerators (PENGs) have shown to be one of the most promising approaches to powering self - sufficient health management systems [4]. These devices transform mechanical energy (movement of the body) into electrical energy [4]. Their capacity to operate in low - energy conditions and deliver continuous power makes them especially interesting because it opens up the prospect of real - time health monitoring without the need for frequent maintenance [4].

The incorporation of nanomaterials into energy - harvesting systems has obtained considerable interest due to the growing need for compact and effective solutions. Due to their superior mechanical, electrical, and piezoelectric qualities, nanomaterials are quickly becoming indispensable in the creation of PENGs of the next generation [4]. Their large surface area, adjustable characteristics, and superior mechanical flexibility make them the perfect choice for improving the longevity and effectiveness of energy - harvesting equipment. Together with improved piezoelectric device performance, these materials provide a solution around bulk materials' drawbacks, such as brittleness and low piezoelectric coefficients. Enhancement of piezoelectric constants enables more effective energy harvesting through atomic - level nanomaterial manufacturing. When altered at the nanoscale, barium zirconate ($BaZrO_3$), one such material, has demonstrated encouraging outcomes because of its significantly large piezoelectric value [5]. The main goal of this project is to improve the piezoelectric constant of $BaZrO_3$ by doping, i. e., $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (x = 0.1, y = 0.05). Further exploration by using density functional theory (DFT) simulations in order to employ it in PENGs for self - powered sensors. Prior to discussing deeply $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (x = 0.1, y = 0.05) using DFT modelling, we must talk about nanomaterials, their kinds, and their uses. Further we have given a glimpse of nanogenerators and their different types.

1.1. Nanomaterials: Types and Applications

Completely different from their bulk counterparts by their unique physical, chemical, and mechanical properties, nanomaterials are identified by their size in the nanoscale (1 - 100 nm) [6]. These features stem from the high surface area to volume ratio and quantum processes, which increases at the nanoscale. Owing to their exceptional properties, nanoparticles are widely employed in numerous industries, including electronics, healthcare, energy, and environmental preservation.

Types of Nanomaterials:
Based on the number of dimensions that constrain them to the nanoscale, nanomaterials can be divided into four categories:

a) Zero - Dimensional (0D) Nanomaterials
All three dimensions of 0D nanomaterials, such as fullerenes, quantum dots, and nanoparticles, are contained inside the nanoscale (less than 100 nm). They are in spherical or nearly spherical shapes. They display unique optical and electrical features as a result of quantum confinement effects. They also have a high ratio of surface area to volume. These materials have several uses; for instance, nanoparticles are utilized in medication delivery, catalysis, and sensors, while quantum dots are used in biological imaging, solar cells, and LEDs [7].

b) One - Dimensional (1D) Nanomaterials

One dimension of 1D nanomaterials is out of the nanoscale, but the other two are contained within it. Among them are nanowires, nanorods, and nanotubes. Their large aspect ratio (length > width) causes it to exhibit anisotropic features. Due to quantum confinement, special mechanical, thermal, and electrical properties exist. Nanocomposites, nanoelectronics, and energy storage all make use of carbon nanotubes (CNTs). Photonic devices, transistors, and nanosensors all use nanowires [7].

c) Two - Dimensional (2D) Nanomaterials

One dimension (thickness) is limited to the nanoscale in 2D nanomaterials, the other two dimensions are outside of it. The greatest examples include nanosheets, graphene, and transition metal dichalcogenides (TMDs). They have adjustable mechanical, optical, and electronic characteristics together with a large surface area. Their in - plane and out - of - plane properties are unique due to their layered nature. Supercapacitors, flexible electronics, and biosensors are only a few of their many uses. Graphene is one example. Field - effect transistors (FETs), spintronic devices, and photocatalysis are exploring the use of TMDs like MoS_2 [7].

d) Three - Dimensional (3D) Nanomaterials

There are no dimensions limited to the nanoscale in three - dimensional nanomaterials. Nanoclusters, nanoporous materials, and nanocomposites are the examples. Its strength - to - weight ratio is great, and they have a big surface area and porosity. Property combinations from 0D, 1D, and 2D nanomaterials can be combined into 3D nanostructures. Biomaterials, energy storage, and structural materials all use nanocomposites, whereas catalysis, gas storage, and separation procedures require nanoporous materials [7].

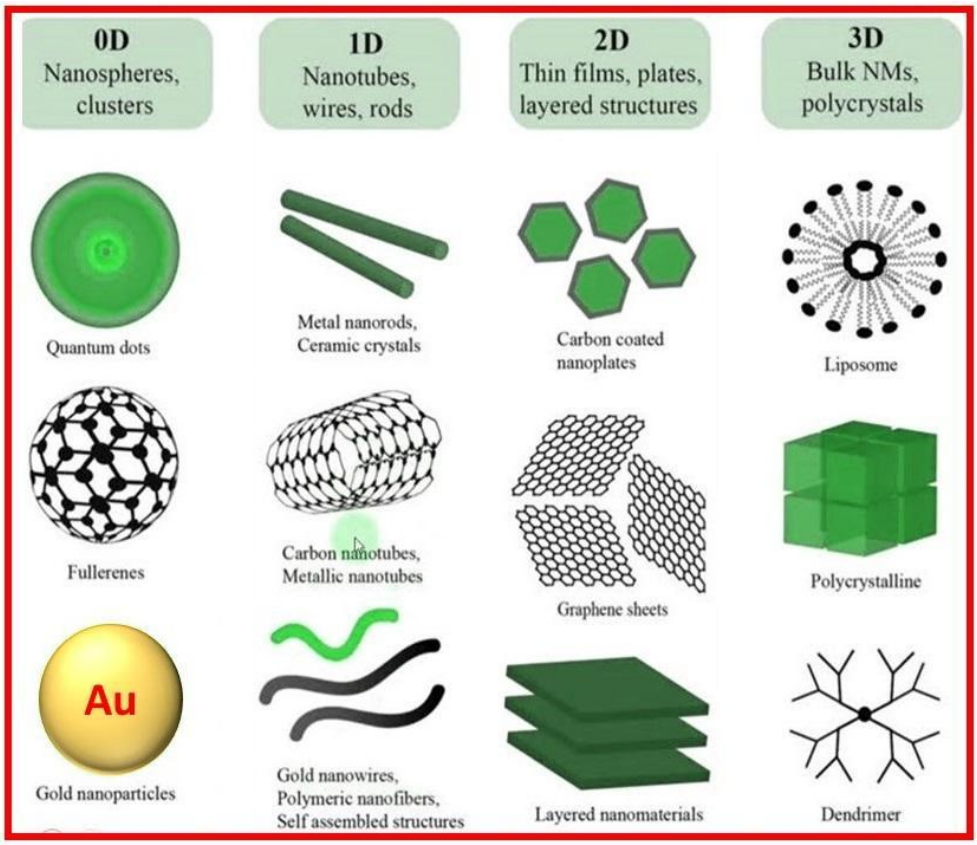

Figure 1: Representation of the different types of nanomaterials including 0D, 1D, 2D and 3D. https: //tinyurl. com/yrb8np7y [7]

Applications of Nanomaterials:

Nanomaterials have completely changed a variety of industries due to their unique characteristics. As specialized drug delivery systems, they are used in medicine to improve treatment efficacy and reduce side effects. Nowadays medicines can be delivered directly to cancer cells using gold nanoparticles. More efficient fuel cells, solar cells, and batteries are produced in the energy industry with the use of nanomaterials. Graphene and carbon nanotubes are being studied for their usage in next - generation energy conversion and storage devices due to their higher conductivity and large surface area. Electronic devices that are more efficient, compact, and quick to operate are made possible by the application of nanomaterials. To facilitate faster and more efficient processing, graphene transistors, for instance, could replace silicon transistors in electronics of the future. Nanoparticles have a high surface area and are reactive, which makes them useful for environmental applications including filtering water and air to remove contaminants [6, 7].

1.2. Nanogenerators: Types and Applications

Nanogenerators use nanomaterials to transform mechanical energy from the surrounding environment into electrical energy. They have become a promising technology that can power sensors and small electronic devices without the use of batteries or other external power sources. Wearable electronics, medical equipment, environmental monitoring systems, and self - powered sensors are just a few of the

many applications for nanogenerators. They improve patient comfort and compliance in the healthcare industry by enabling continuous health monitoring without the need for regular battery replacements. Nanogenerators provide real - time data for preventive measures by powering sensors that identify pollution levels, climatic changes, and natural disasters in the environment. Nanogenerators can power wearable electronics, which lessens the need for regular recharging and improves user experience. This applies to consumer electronics. Wearables and accessories such as fitness trackers and smartwatches can be powered by PENGs, which are devices that use body movement to generate energy. To enhance productivity and avoid malfunctions, industrial environments can employ nanogenerators to supply power to wireless sensors that keep an eye on equipment and infrastructure [8].

Types of Nanogenerators:

a) Piezoelectric Nanogenerators (PENGs):
It uses the piezoelectric effect, which occurs when mechanical stress causes some materials to become electrically charged. PENGs are useful for capturing mechanical energy from vibrations, body motions, and other mechanically - occurring environments [8].

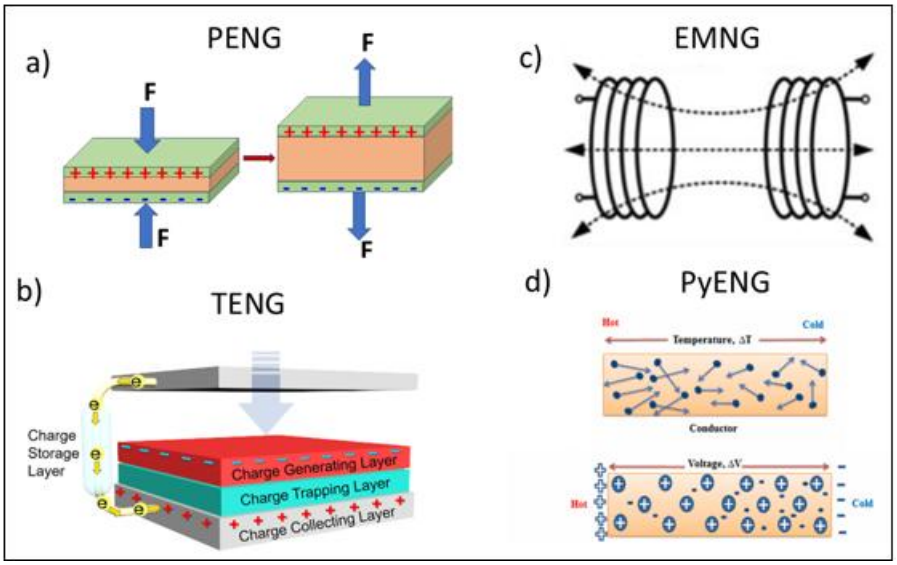

Figure 2: Schematics of working principle of different types of nanogenerators (https: //doi. org/10.1038/s41427 - 019 - 0176 - 0, https: //doi. org/10.1016/j. nanoen.2021.105888).

b) Triboelectric Nanogenerators (TENGs):
The triboelectric phenomenon, which produces electric charge when two materials come into contact and separate. TENGs gets energy from motion, including typing, walking, and vibrations [8].

c) Pyroelectric Nanogenerators (PyENGs):
It uses the pyroelectric phenomenon to transform temperature into electrical energy. They are appropriate for obtaining energy from waste heat [8].

d) Electromagnetic Nanogenerators (EMNGs):
It us used to turn mechanical motions into electricity by using electromagnetic induction. To increase energy output, they are frequently combined with other nanogenerators [8].

Piezoelectric Nanogenerators (PENGs)
PENGs are a particularly notable form of nanogenerator because of its great efficiency and ability to directly convert mechanical energy into electrical energy via the piezoelectric effect. PENGs are particularly appealing for health monitoring applications due to their ability to harvest energy from low - frequency and low - amplitude mechanical movements, like those of the human body. These PENGs display the piezoelectric effect. Because of this feature, PENGs are perfect for incorporating into wearable technology that can continuously monitor health metrics like vital signs without the use of external power sources. Their exceptional sensitivity and dependability make them even more ideal for precise and accurate health monitoring [8].

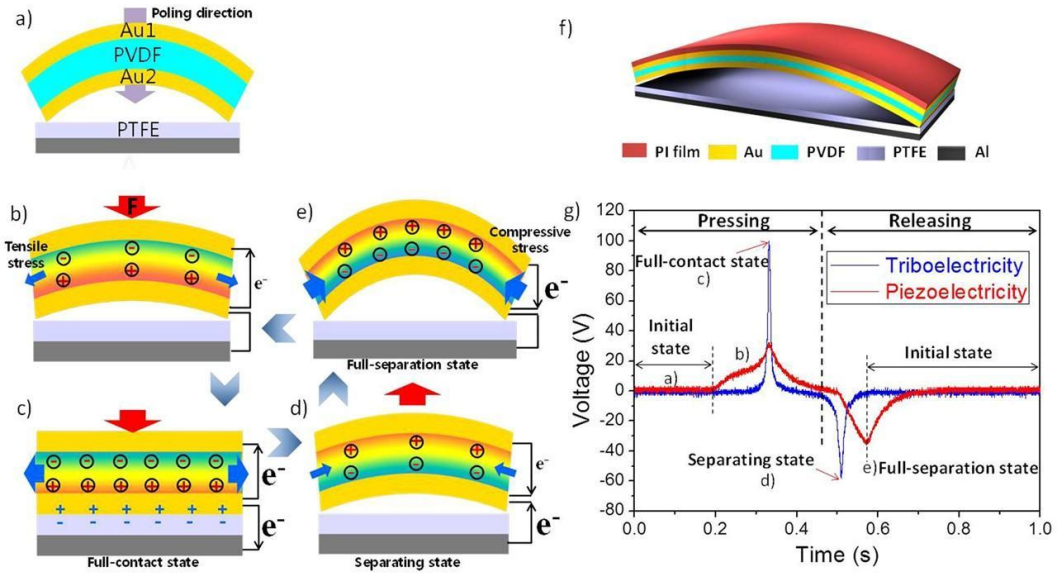

Figure 3: Schematics of the working principle of PENGs (https: //doi. org/10.1038/srep09309).

Apart from health monitoring, PENGs are used in numerous other domains. Microelectromechanical systems (MEMS) are tiny devices that integrate mechanical and electrical components. They can be powered by them. MEMS are employed in many different applications, including as medical equipment and automobile sensors. PENGs can also be used in environmental monitoring, where they can power sensors that track the quality of the air and water by harnessing energy from vibrations or wind.

1.3. Piezoelectric Materials

When subjected to mechanical stress, piezoelectric materials can produce electrical charges [9, 10]. Because of this characteristic, they are essential in many different applications, including energy - harvesting devices, actuators, and sensors. Because the piezoelectric effect is bidirectional, these materials can be used for both sensing and actuation. Specifically, supplying an electrical field can also cause mechanical strain. Perovskites, wurtzites, and some polymers are examples of materials with piezoelectric properties that come in a variety of crystal forms. Quartz (SiO_2), zinc oxide (ZnO), lead zirconate titanate (PZT), and barium titanate ($BaTiO_3$) are among the minerals that demonstrate piezoelectric behavior [11, 12, 13]. Many of these materials do, however, have drawbacks, such as inadequate piezoelectric constants or toxicity (in the case of lead - based compounds). Perovskite material barium zirconate ($BaZrO_3$) is becoming more and more popular because of its favorable environmental profile and, when doped properly, high piezoelectric constant. We concentrate on $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ for this research because it has been reported that $Ba_{0.85}Ca_{0.15}Zr_{0.9}Ti_{0.1}O_3$ exhibits a high piezoelectric constant of d_{33} = 650 pC/N [5]. To further improve this composition's piezoelectric qualities, we have decided to dope it with Sr and Sn (x = 0.1 and y = 0.05). $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ was selected because doping in perovskite structures enables the adjustment of their mechanical and electrical characteristics. Improved polarization can result from the presence of Sr and Sn in the lattice, and this directly affects the piezoelectric constant d_{33}. Greater efficiency in transferring mechanical energy into electrical energy is indicated by a higher d_{33} value, which makes the material more appropriate for PENG applications. We seek to determine the effects of adding Sr and Sn on this materials piezoelectric characteristics using first - principles techniques, namely density functional theory (DFT).

Types of Piezoelectric Materials for PENGs

The selection of piezoelectric materials has a major impact on PENGs performance. Piezoelectric capabilities are shown by a variety of materials; choosing the best material is essential to increasing PENGs energy harvesting effectiveness.

Common Piezoelectric Materials:

a) **Lead Zirconate Titanate (PZT):**
A popular piezoelectric ceramic that offers exceptional energy conversion efficiency and high piezoelectric coefficients. Nevertheless, it is less environmentally beneficial due to the lead content.

b) **Barium Titanate ($BaTiO_3$):**
A low - impact substitute for PZT that has a high dielectric constant and good piezoelectric qualities. It is frequently utilized in sensors and capacitors.

c) **Zinc Oxide (ZnO):**
A transparent, flexible PENG - suitable piezoelectric semiconductor with good piezoelectric characteristics and nanostructure - forming capabilities.

d) **Polyvinylidene Fluoride (PVDF):**
An excellent choice for wearable and implanted PENGs is a flexible, lightweight, and biocompatible piezoelectric polymer.

e) **Gallium Nitride (GaN):**
Useful in high - frequency and high - power applications, this high - performance piezoelectric material has exceptional mechanical and thermal stability.

f) **Barium zirconate ($Ba_{1-x}Ca_xZr_{1-x}Ti_xO_3$):**
The material exhibits great potential for PENGs because of its notably high piezoelectric constant value. Barium zirconate is a versatile material with many uses because of its excellent mechanical stability and ability to be produced as nanoparticles.

Piezoelectric Material for current study
Doped Barium zirconate $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (x = 0.1 and y = 0.05) is selected for this investigation from among these materials because of its superior ferroelectric qualities, mechanical stability, and piezoelectric qualities. Due to its effectiveness and adaptability, barium zirconate is a good option for creating effective PENGs for self - powered health monitoring sensors. Due to its dual ferroelectric and piezoelectric characteristics, doped barium zirconate can be useful for devices with multiple uses. Because of its mechanical stability, PENGs can be designed with greater flexibility because of its capacity to develop various morphologies. It is the perfect material for creating high - performance PENGs because of these qualities.

2. Simulation Method:

2.1. First Principle Theory

First - principle theory or ab initio theory [14], describes computing techniques that start with fundamental quantum mechanical principles and work their way up to material qualities without the need for empirical parameters. By solving the Schrödinger equation to explain how electrons and nuclei behave inside a system, the technique is said to be "first - principle" based. The first - principle method most frequently employed in condensed matter physics and materials research is Density Functional Theory (DFT) [15]. In order to facilitate the efficient calculation of features like electronic structure, polarization, and magnetism, DFT represents the system's energy as a functional of the electron density, therefore simplifying the many - body problem of interacting electrons. This is crucial tool in the design of semiconductors, nanomaterials, and energy - harvesting materials like piezoelectrics because of their exceptional utility for atomic - level material research. This is now essential for material design and optimization, which includes figuring out how doping and structural changes will affect the material's performance.

Using DFT, we can accurately predict the piezoelectric constant d_{33} and learn more about how doping affects the atomic arrangement and electrical characteristics. Moreover, DFT can be used to determine a piezoelectric nanogenerator's output voltage, which yields important data for maximizing its efficiency. In order to determine the piezoelectric constant of the $Ba_{1-x}Ca_xSr_yZr_{1-x}Ti_xSn_yO_3$ (x = 0.1 and y = 0.05) structure, we simulated it using DFT in this study. Pseudopotentials and plane - wave basis sets were used in the simulation to simulate the core - electron interactions. For the computations, the Perdew - Burke - Ernzerhof (PBE) exchange - correlation functional was used. Prior to computing the d_{33} value, the structure was adjusted to reduce the overall energy. We anticipate that the increased lattice distortion and polarization caused by the doping of Sr and Sn will result in an increase in piezoelectric response. Furthermore, we performed a simulation of the $Ba_{1-x}Ca_xSr_yZr_{1-x}Ti_xSn_yO_3$ - based PENGs output voltage under mechanical strain. By calculating the voltage using the applied stress and the piezoelectric constant, the materials potential for energy harvesting was estimated.

3. Results and Discussion

$BaZrO_3$, a perovskite material, is a preferred candidate for a variety of piezoelectric applications because of its massive ionic displacements, high dielectric constant, and notable lattice distortions when doped. The ability to precisely adjust the structure at the atomic level in order to generate lattice instabilities and improve polarization is the primary rationale for choosing $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (with x = 0.1, y = 0.05). $BaZrO_3$ has a relatively low piezoelectric constant when it is pure. Nevertheless, we were able to create structural distortions and alter the electric dipole alignment, which results in improved piezoelectric performance, by replacing Ca, Sr, Ti, and Sn into particular lattice places. The piezoelectric capabilities of perovskite oxides, such as $BaZrO_3$, are directly related to the displacement of the cations, such as Ba, Zr, etc., and the polarization vector shift that follows. Doping the material increases these displacements. Specifically, Zr - O bond lengths are changed and extra lattice strains are induced by the doping of Sr and Sn.

A - site of the perovskite lattice is occupied by Ba ions in the structure of $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$, whereas B - site is occupied by Zr ions. Since the ionic radii of Sr and Ca are less than those of Ba, their replacement into the A - site leads to localized distortions. A decreased lattice constant caused by this discrepancy in ionic radii causes strain in the material. The B - site additions of Ti and Sn have an impact on the d - orbital hybridization process with oxygen. The polarization is enhanced by Ti greater propensity to create off - center displacements. Alternatively, Sn alters the electronic structure, resulting in improved interaction between polarization and lattice distortions. Increasing the piezoelectric coefficient d_{33}, one of the material's key performance metrics in energy harvesting applications, depends on this structural adjustment.

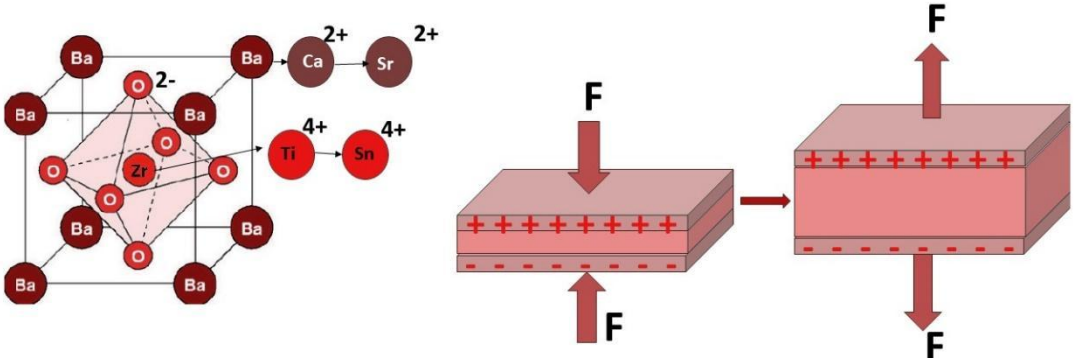

Figure 4: Schematics of the crystal structure and piezoelectric effect in $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (with x = 0.1, y = 0.05)

3.1. Simulation Results

We used DFT to quantitatively evaluate the piezoelectric characteristics of $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (x = 0.1, y = 0.05). The PBE generalized gradient approximation (GGA), which is renowned for precisely modelling electronic characteristics while maintaining computing efficiency, was used to do the DFT computations. To explain the core - electron interactions in this study, we used projector - augmented wave (PAW) pseudopotentials and plane - wave basis sets. The simulation started with the goal of decreasing the total energy and optimizing the crystal structure of $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$. The conjugate gradient approach, which modifies atomic locations until the forces acting on all atoms fall below a given threshold, was used to accomplish this. Considerable lattice aberrations were visible in the optimized structure, especially in the Zr - O bond lengths. These distortions affect the polarization of the material, which is important for improving the piezoelectric response. Additionally, the ZrO_6 octahedra exhibits an asymmetric tilting, which is discovered by structural optimization and adds to the unit cell net dipole moment. After the structure was adjusted, density functional perturbation theory (DFPT) was used to compute the piezoelectric tensor. This technique makes it possible to calculate linear reactions to an external strain, like polarization. A d_{33} value of 830 pC/N was found by the DFPT calculations, which is a considerable improvement over the much lower piezoelectric constant of the undoped $BaZrO_3$. The combined effects of ionic displacements, lattice distortion, and higher polarization from Sr and Sn doping are responsible for the increased d_{33}.

Output Voltage for PENG

We first calculated the improved piezoelectric constant and then the output voltage produced under mechanical strain by the $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ based PENG. The PENG model simulates conditions similar to human motion by assuming that the material is subjected to periodic mechanical stress. The following relationship controls a piezoelectric materials output voltage.:

$$V = d_{33} \cdot F \cdot h / \varepsilon_0 \cdot A$$

where

- V is the output voltage,
- d_{33} is the piezoelectric constant (in this case, 830 pC/N),
- F is the applied force (mechanical strain),
- h is the thickness of the piezoelectric material,
- ε_0 is the permittivity of free space, and
- A is the surface area of the material.

The nanomaterial $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ was used in this simulation, with a particle size of 500 nm. The applied force was selected to simulate low - frequency mechanical stress, such as that caused by human motion. For the PENG device, the DFT - based calculations anticipated an output voltage of roughly 18 V, which is a major improvement over conventional materials used in similar applications. The improved piezoelectric constant, which directly affects the quantity of charge created in response to mechanical stress, is responsible for the greater output voltage. Realistic and scalable output voltages for practical applications were guaranteed by the simulation's consideration of the impacts of boundary conditions and material geometry. Dielectric loss can occasionally lower the efficiency of energy conversion, hence the impact of dielectric characteristics on the output voltage was also taken into account. On the other hand, the addition of Sr and Sn doping to the $BaZrO_3$ matrix resulted in a greater output voltage by decreasing dielectric losses and improving the piezoelectric response.

The improved piezoelectric constant and considerable output voltage of $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ make it a highly attractive material for PENG applications, according to the results of our DFT - based calculations. This material's unique properties, including strain engineering, polarization effects, and lattice distortions, make it ideal for self - powered sensors found in health monitoring systems. Subsequent research endeavors will center around verifying these findings through experiments and refining the substance for certain uses. Further experimental studies are required to validate this result.

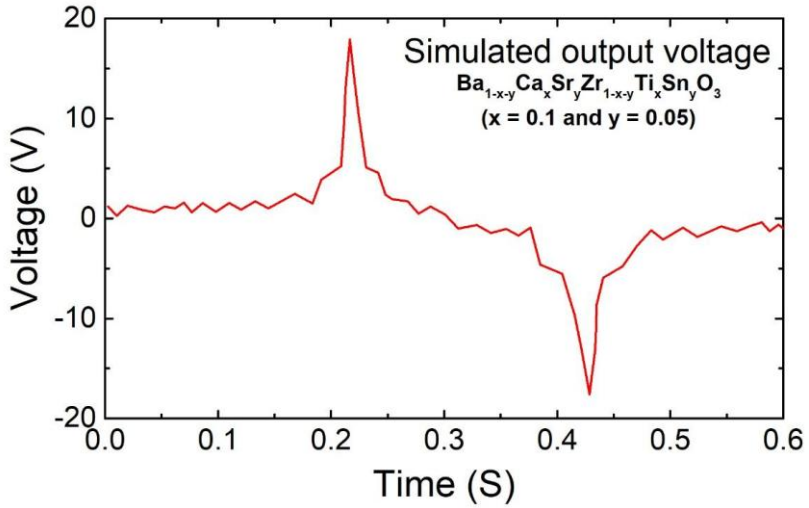

Figure 5: Simulated output voltage for $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (x = 0.1 and y = 0.05) based nanogenerators.

4. Conclusion

In this work, we used DFT to examine the piezoelectric properties of the $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ (x = 0.1 and y = 0.05) material. The material was chosen because of its potential for further doping augmentation and its claimed high piezoelectric constant. According to our models, adding Sr and Sn to the $BaZrO_3$ lattice enhances piezoelectric performance, as seen by a rise in the d33 value. Furthermore, this material's potential for producing sizable output voltages under mechanical strain was shown by the simulation of the PENG based on it. This makes the material a promising option for self - powered sensors, which may find extensive usage in health monitoring, where constant power is necessary for the acquisition of real - time data. Conclusively, the $Ba_{1-x-y}Ca_xSr_yZr_{1-x-y}Ti_xSn_yO_3$ material exhibits great potential as an extremely effective piezoelectric material for applications involving energy harvesting. Important insights into the material's piezoelectric characteristics and its possible integration into PENGs for powering wearable and implantable sensors were gained through the use of first - principle simulations, especially DFT. The creation of prototype devices based on this material and the experimental validation of the simulation results will be the main areas of future investigation.

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