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Study of Piezoelectric Properties of Barium Titanate for Energy Harvesting System Using COMSOL

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Abstract: The conversion of mechanical energy created by environmental vibrations into electrical energy is the main advantage of piezoelectric materials. An energy harvester with the help of photoelectric sensor using non-toxic Barium titanate is studied and a model of energy harvester unit is simulated in COMSOL multiphysics software package. This simulation of piezoelectric sensor to detect environmental vibration through rolling noise are investigated and compared for different frequency. In common practices, the rolling noise induces sound wave in the railway track. This rolling noise is a wave which is useless in nature. But, this unwanted rolling noise may be used in a transducer to convert the unwanted form of energy to useful electrical form of energy. In the new era of science, the new ideas about induction of new form energy without harming the environment are needed. This paper is dedicated to use of non- toxic Barium titanate in place of toxic lead zirconate titanate (PZT). In order to improve the performances of the energy harvester, the geometry of the model has to be properly designed. Different geometries were investigated using simulation. The results of simulations are used to find optimum geometry and size of Barium titanate used to develop the main unit of energy harvester. The rail wheel interaction results rolling noise in the railway track. This rolling noise is dynamic in nature. These sound waves can move in the railway track with high speed. The piezoelectric transducers receive the wave and induce electric current. This induced electrical energy can be stored for future use with the help of batteries. These induced electrical energy as well as stored electrical energy may be used to operate various electrical and electronics equipment in the absence of conventional electrical energy.

Keywords: Piezoelectric Material, Energy Harvesting, Barium Titanate, Rolling Noise

1. Introduction

The Study of *Piezoelectric* material is the key issue of researcher due to its extraordinary behavior. One of the authors, Dr. Shuchitangshu Chatterjee has done extensive work on piezoresistive/piezoelectric effect on galena aggregate and galena concentrate early in 1990's and designed Pressure transducer which is commercialized on February 3, 1994 [1-5]. Piezoelectricity in Barium Titanate ($BaTiO_3$) is ability of material to induce an electric potential in response to applied mechanical stress [6]. Barium titanate is a member of perovskite family. The lattice constant of crystal of perovskite family is about 4 A°. due to rigidity of oxygen octahedral network and ionic radius of oxygen (1.35A°) [7]. Barium titanate has an additional advantage due to its perovskite structure. Many different cations can be substituted on Ba – ions as well as Ti –ions without changing in overall structure. So, it is possible to redefine the general material properties like dielectric constant, curie temperature etc. with a simple substitution of a different cation. Generally, the unit cell of Barium Titanate has cubic symmetry at temperature greater than curie temperature (about 120°C) upto 1460°C [8]. Due to anomalous polarization effects in barium titanate, it has interesting piezoelectric properties [8-10]. Lead zirconate- Titanate (PZT) is most popular piezoelectric material widely used in commercial product. But, the toxicity of lead is a vital factor which prevents the use of PZT in commercial products.

Europian union introduced regulations, Restriction of Hazardous substance (ROHS) Directive 2002/95/EC and ROHS Directives (2015/863/EU) regarding use of Lead (Pb) and other toxic elements in commercial product [10]. These restrictions have stimulated the work of researcher in the field of lead free piezoelectric material like Barium Titanate. The piezoelectric materials can be easily used for energy harvesting from vibrational source. It can efficiently convert mechanical strain to an electric charge without external source of energy [11]. Barium Titanate is a lead (Pb) free piezoelectric material which has capability to fabricate at different scale. In this paper, we have presented the study of piezoelectric behaviour of Barium Titanate over a frequency range 50 Hz- 500 Hz which may be created by vibration due to rolling noise. The study shows highly considerable variation in the frequency range 75Hz – 150Hz. So, we have concentrated the study in the frequency range 75Hz – 150 Hz. We studied the Total energy and power dissipation in that frequency range along with terminal current and terminal voltage using a simulation software COMSOL Multiphysics. COMSOL Multiphysics is a software package used to simulate different designs to find numerical solution.

2. Model Geometry

In Simulation software, Comsol Multiphysics, the real situation is modelled under same boundary conditions. In this paper we have to design a transducer using non-toxic piezoelectric material, Barium titanate of dimension 8mm x 6 mm x 1.42mm to induce piezoelectric current using rolling noice. So, in this simulation, a steel block of dimension 20mm x 18mm x 5 mm is considered as the base for rolling noise. The properties of steel are given in Table 1. A hole of size 12mm x 10mm x 5mm is drilled at the center of the base slab. This hole is drilled to fit an arrangement of transducer which can receive the rolling noise from steel base. A rectangular ring of nylon of thickness 2mm is fixed in the hole. The properties of nylon are shown in Table 1. Nylon behaves as shock absorber as well as insulator. The experimental material ($BaTiO_3$) along with two electrodes of aluminium [Layer 1 (Al) – 1.7 mm, Layer 2 ($BaTiO_3$) - 1.6mm, Layer 3 (Al) -1.7mm] is fixed in the vacant space of the slab. The property of Aluminium and Barium Titanate is in Table 1 and Table 2 respectively. The model is shown in Figure 1. The hypothetical model for simulation is shown in Figure 1.

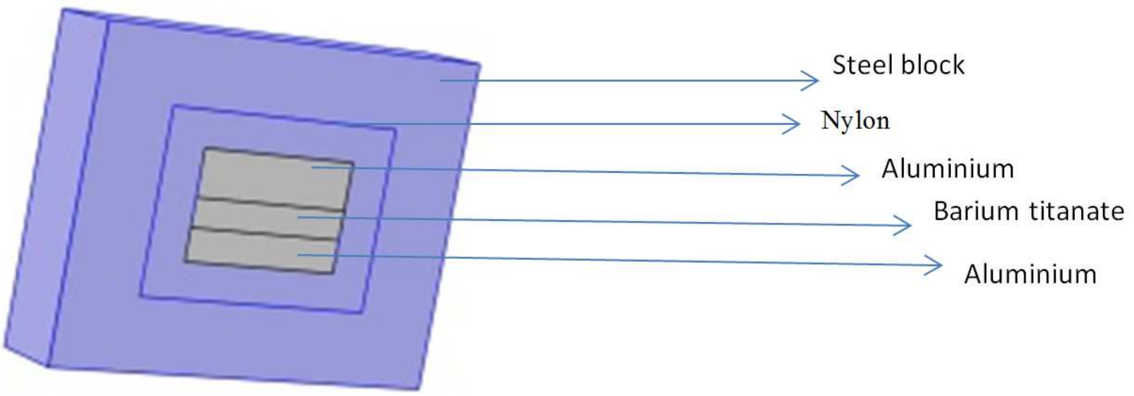

Figure 1. *The model designed to study the piezoelectric properties of Barium titanate and to design the energy harvesting system.*

2.1. Physical Properties of Materials Used in the Model of Piezoelectric Energy Harvesting System

In this model, we have used Barium titanate (piezoelectric material), Aluminium (terminals), Nylon (Insulator as well as shock absorber) and Steel (Base for energy harvesting system, may be a railway track or other devices). The well-known standard values of useful parameters like Density, Young modulus, Poisson’s ratio, thermal conductivity, electrical conductivity, relative permittivity, heat capacity at constant pressure, etc is collected by us to use in the simulation.

Quantitative Properties of Steel, Nylon and Aluminium: The standared values of useful parameters are shown in Table 1.

Table 1. *Properties of Steel, Nylon and Aluminium Source: COMSOL Multiphysics, and NIST Website, www.nist.gov.*

Property	Steel	Nylon	Aluminium
Density	7850 Kg/m^3	1150 Kg/m^3	2700 Kg/m^3
Young Modulus	$2x10^{11}$ Pa	$2x10^9$ Pa	$7x10^{10}$ Pa
Poisson’s ratio	0.30	0.40	0.33
Relative permeability	1		1
Heat capacity at constant pressure	475 J/(Kg. K)	1700 J/(Kg. K)	900 J/(Kg. K)
Thermal conductivity	44.5 W/(m.K)	0.26 W/(m.K)	238 W/(m.K)
Electrical conductivity	4.032×10^6 s/m	4.032×10^6 s/m	3.774×10^7 s/m
Relative permitivity	1	1	1
Co-efficient of thermal Expansion	$1.23 \times 10^{-6} K^{-1}$	$2.8 \times 10^{-4} K^{-1}$	$2.3 \times 10^{-5} K^{-1}$

2.2. Properties of Barium Titanate

The comsol multiphysics work on the Finite Element Method (FEM). The finite element method for simulation of piezoelectric effect requires the matrix representation of physical quantities to apply Constitutive Relations. The following variables are significantly used in constitutive equation for piezoelectric effects.

Table 2. *Description of variables used in constitutive equation used in COMSOL Multiphysics.*

Symbol	Description	Type	Size	unit
D	Electric charge density	Vector	3 x 1	C/m^2
E	Applied Electric field	Vector	3 x 1	V/m
s	Strain component	Vector	6 x 1	Unit less
T	Stress component	Vector	6 x 1	N/m^2
S	Compliance coefficient	Matrix	6 x 6	m^2/N
C	Stiffness	Matrix	6 x 6	N/m^2
ε	Electric permittivity	Matrix	3 x 3	F/m
d	Coupling coefficient	Matrix	3 x 6	C/N

2.3. Matrix/Vector Used in Simulation

The following matrix/vector used in simulation is developed by author 1 with the help of data collected from ready data of COMSOL Multiphysics software and the document published by COMSOL, https://doc.comsol.com/5.5/doc/com.comsol.help.sme/sme_ug_theory.06.23.html. A. C. Dent, R. Stevens and C. R. Bowen of Materials Research Centre, Department of Mechanical Engineering, University of Bath, Bath BA2 7AY, UK with M. G. Cain & M. Stewart of National Physical Laboratory, Teddington, Middlesex TW1 OLW, UK published a paper on Effective elastic properties for unpoled barium titanate [12]. This paper along with other recent papers on Barium titanate helped the author to design the matrix regarding elastic properties of barium titanate [12, 13]. The description about the nature, unit and size of variable used in simulation is shown in Table 3.

Table 3. *Properties of Barium titanate, Source: COMSOL Multiphysics.*

Property	Value	unit	Remarks
Density	**6220**	**Kg/m^3**	
Elasticity matrix,	$\begin{bmatrix} 8.05 & -2.35 & 8.05 & 0 & 0 & 0 \\ 0 & -5.24 & -5.24 & 0 & 0 & 0 \\ 0 & 0 & 1.57 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.84 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.84 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8.84 \end{bmatrix} x10^{-11}$	Pa	Stress-charge form
Coupling matrix,	$\begin{bmatrix} 0 & 0 & -2.69289 & 0 & 0 & 0 \\ 0 & 0 & -2.69289 & 0 & 0 & 0 \\ 0 & 0 & 3.65468 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 21.3043 & 0 \\ 0 & 0 & 0 & 21.3043 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} x10^{-11}$	C/m²	Stress-charge form
Relative permittivity	$\begin{bmatrix} 1976.8 & 0 & 0 \\ 0 & 1976.8 & 0 \\ 0 & 0 & 111.7 \end{bmatrix}$		Stress-charge form
Compliance matrix,	$\begin{bmatrix} 8.05 & -2.35 & 8.05 & 0 & 0 & 0 \\ 0 & -5.24 & -5.24 & 0 & 0 & 0 \\ 0 & 0 & 1.57 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.84 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.84 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8.84 \end{bmatrix} x10^{-11}$	1/Pa	Strain-charge form
Coupling matrix,	$\begin{bmatrix} 0 & 0 & -3.45 & 0 & 0 & 0 \\ 0 & 0 & -3.45 & 0 & 0 & 0 \\ 0 & 0 & 8.56 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.92 & 0 & 0 \\ 0 & 0 & 0 & 3.92 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	C/N	Strain-charge form
Relative permittivity	$\begin{bmatrix} 2920 & 0 & 0 \\ 0 & 2920, & 0 \\ 0 & 0 & 168 \end{bmatrix}$		Strain-charge form

3. Piezo Electric Energy Harvesting System

The piezoelectric energy harvesting system is designed by using three subunits.

a. Energy harvesting unit, b. Vibration control unit and c. Harvester control unit.

3.1. Energy Harvesting Unit

The energy harvesting unit consists of a source of vibration and a transducer. The transducer changes the vibrational energy to other form of energy.

3.2. Vibration Control Unit

The Vibration control unit consists of accelerometer and frequency tuning actuator. The accelerometer is a device used for the independent measurement of the vibrational source such that the damping and resonant frequency can be studied. On the other hand frequency tuning actuator is used to tune the frequency of transducer such that the maximum energy can be harvested.

3.3. Harvester Control Unit

The harvester control unit consists of Electrical energy storage device like Battery, voltage regulation devices (electronic circuit) and computational load. The computational load is scheduling mechanism based device. It is used to send a signal to the harvester control regarding load on the system.

These subunits may be compiled to get a complete system of energy harvesting using piezo electricity. The block diagram for functional description of a model of piezoelectric energy harvesting system is shown in Figure 2.

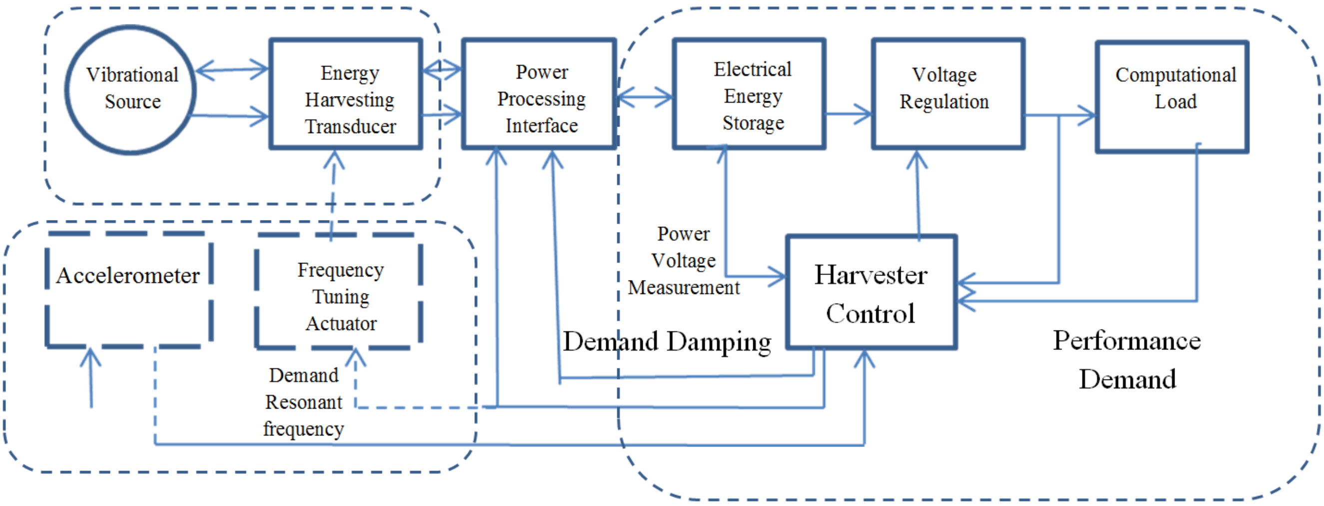

Figure 2. *Block diagram of Piezoelectric Harvesting System [11, 14, 15].*

In 2009, Shashank Priya, Daiel J Inman highlighted the cohesive overview of fundamentals of Energy Harvesting System based on piezoelectric, electromagnetic and thermo electric technique with current scenario [16]. This volume of book helped the author to design piezoelectric harvesting system. A number of recent papers have been published in this research field. But, our study is concentrated to the impact of replacement of toxic piezoelectric material (like Lead zirconate- Titanate, PZT) by non-toxic piezoelectric material, Barium titanate (BT).

4. Piezoelectric Constitutive Relation (Used in COMSOL Multiphysics)

The Comsol Multiphysics Software is a package for scientific simulation. It is based on Finite Element Method (FEM). It is a used for the numerical solution of various scientific problems based on different simulation condition. A number of research papers have been published using this package. Buethe and C. P. Frizen designed the active sensor using this package and validated the results by experimental data [17]. M. Guizzetti simulated a piezoelectric energy converter [18]. Generally, in mechanical problems, a constitutive equation describes the effect on strain with respect to applied stress on the material or vice-versa. The general constitutive equations in mechanical problem is $S = s\sigma$; Where S is strain on the material, s - Compliance, σ - Stress. On the other hand, in electrical problems, Constitutive equations describe the nature of movement of charge in a (dielectric) material when it is subjected to a voltage, or vice-versa. The general constitutive equations in electrical problem is $D = \varepsilon E$; Where D – Electric Displacement, ε - Permiability, E – Electric field. Piezoelectric materials are concerned with electric properties as well as mechanical properties. Thus Piezoelectric materials combine two seemingly dissimilar constitutive equations into one coupled equation, written as:

$$S = s_E.\sigma + d^t. E$$

$$D = \varepsilon_T. E + d^C.\sigma$$

Where, d is coupling matrix.

In the comsol Multiphysics software the same constitutive equation is used. In matrix form we can write the constitutive equation which has been used in software for study of piezoelectric behaviour of Barium titanate as follow:

$$D_i = e^{\sigma}{}_{ij}\, E_j + d^{d}{}_{im}\, \sigma_m$$

$$\varepsilon_k = d^{c}{}_{jk}\, E_j + s^{E}{}_{km}\, \sigma_m$$

Where

D: Electric Displacement matrix (3x1) in coul/m^2;

ε: Strain vector (6x1), It is dimension less physical quantity;

E: Applied Electric field vector (3x1) in Volt/m;

σ_m: Stress vector (3x1) in N/m^2;

$e_{ij}{}^{\sigma}$: Dielectric permittivity (3x3) in Farad/m;

$d_{im}{}^{d}$: Piezoelectric coefficient (3x6) in C/N, electric displacement per unit stress at constant electric field. d stands for direct piezoelectric effect;

$d_{jk}{}^{c}$: Piezoelectric coefficient (6x3) in m/volt, electric displacement per unit Electric field at constant Stress. c stands for converse piezoelectric effect;

$S^{E}{}_{km}$: Dielectric compliance (6x6) in m^2/N;

The coefficient $d_{im}{}^{d}$ and $d_{jk}{}^{c}$ are numerically equal. [18]

5. Simulation Through Comsol Multiphysics

Simulation using comsol Multiphysics for circular -shaped PZT-5H sensor was done by S. Kumar and Y. K jain in 2015 [19]. The results are impressive. On the other hand a comprehensive review on the state-of-the-art of piezoelectric energy harvesting is reported by Nurettin Sezer and Muammer koc in 2021 [20].

In this simulation, we have selected three different physics used in comsol multiphysics software –Solid mechanics, Electrostatics and piezoelectricity.

Solid mechanics was used to study the vibrational behaviour of rolling noise in steel beam (It may be railway track for energy harvesting from railway track) which is the medium to pass vibration to piezoelectric sensors.

Electrostatics was used to observe the potential difference between terminals of sensors (floating and ground terminals). The mode of study was frequency dependent. The piezoelectric sensor was designed by Barium titanate Material backed by nylon. This nylon was not only a support. It was also used as an efficient damper for back travelling pressure wave. The selection of boundary conditions of physics in model is very important for correct result. We have selected the boundary conditions associated with piezoelectricity, structural mechanics and Electrostatics.

Meshing is an important part of simulation in Comsol Multiphysics package. It is one of the key components of software to obtain accurate results from an FEA model. Generally, the smaller mesh size provides more accurate solution as the designs are better sampled across the physical domains. The high aspect ratio of the modelled geometry makes the problem numerically challenging. There is only a short moderated range of mesh size where the result has much reliable. Outside this range of mesh size (too coarse or fine) the result is not reliable. We have used the mesh size range 0.002 – 0.02. Meshed model is shown in Figure 3.

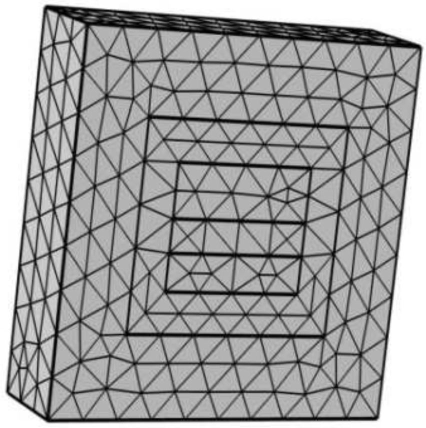

Figure 3. *The model is meshed to find the result.*

6. Results and Discussion

We have studied the simulated result in following parameters.

6.1. Frequency Response for Voltage and Power

We have studied the variation of voltage, mechanical power and electrical power with respect to frequency in comsol multiphysics. The input mechanical power (in mW) and the output harvested power (in mW) as well as the induced potential difference between terminals of piezoelectric material, Barium titanate (in volt) vs. excitation frequency is shown in Figure 4. The load impedance is 12 KΩ. The graph is auto generated by the software as per specification of project. The slope of voltage curve with respect to change in excitation frequency is considerable high between 100Hz – 120 Hz. The voltage is more than 2.4 volt between 105 Hz – 110 Hz. The variation of input mechanical power with frequency coincides with the variation of output electrical power. They are at the maximum value in between 100Hz - 110 Hz.

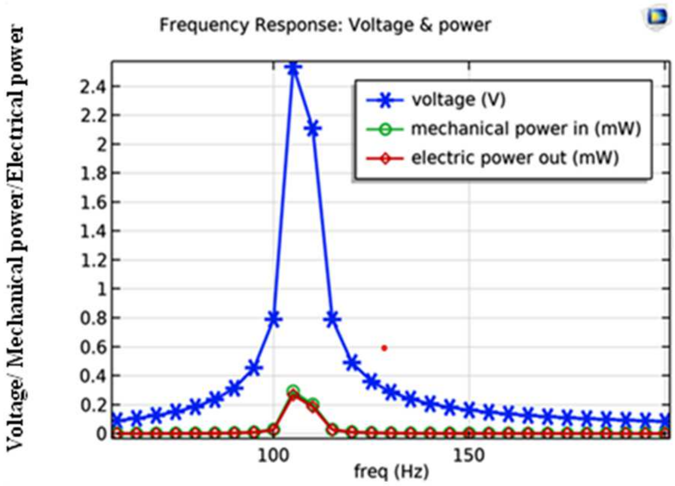

Figure 4. *The input mechanical power (in mW), the output harvested power (in mW) and the induced potential difference between terminals of piezoelectric material, Barium titanate (in volt) vs. excitation frequency.*

6.2. Total Energy and Power Dissipation w.r.t Variation in Frequency

Total energy and power dissipation at different frequencies was calculated using the software package. The experimental value of total energy (in joule) and the power dissipation during the process of piezoelectric energy harvesting (in mW) is shown in Table 4. According to observed data total Energy is maximum (4.5438 x10^{-7} Joule) at frequency 105 Hz. In the addition with this result, the power dissipation is maximum (0.0016883 mW) at 105 Hz.

Table 4. *Variation of Total Energy and power dissipation w.r.t frequency.*

Frequency (Hz)	Total energy J	Power dissipation mW
75.000	3.1351x10^{-9}	8.4660 x10^{-6}
80.000	4.1708 x10^{-9}	1.1984 x10^{-5}
85.000	5.9520 x10^{-9}	1.8123 x10^{-5}
90.000	9.4308 x10^{-9}	3.0319 x10^{-5}
95.000	1.7837 x10^{-8}	6.0349 x10^{-5}
100.00	4.8533 x10^{-8}	1.7231 x10^{-4}
105.00	4.5438 x10^{-7}	0.0016883
110.00	2.8750 x10^{-7}	0.0011153
115.00	3.6848 x10^{-8}	1.4891 x10^{-4}
120.00	1.3164 x10^{-8}	5.5302 x10^{-5}
125.00	6.5443 x10^{-9}	2.8527 x10^{-5}
130.00	3.8379 x10^{-9}	1.7329 x10^{-5}
135.00	2.4865 x10^{-9}	1.1610 x10^{-5}
140.00	1.7220 x10^{-9}	8.3018 x10^{-6}
145.00	1.2514E-9	6.2201 x10^{-6}
150.00	9.4300 x10^{-10}	4.8264 x10^{-6}

The total energy (in µJ) vs, excitation frequency (within frequency range 75 Hz - 150 Hz) is plotted using MATLAB. The graph is shown in Figure 5. The maximum harvested energy is 0.45438 µJ at excitation frequency 105 Hz. The Energy is effectively high between 105 Hz - 110 Hz. Thus the piezoelectric harvester using Barium titanate works well in rolling noise having frequency between (105 Hz - 110 Hz). The power dissipation during the energy harvesting process (using piezoelectric material, Barium titanate) is an important factor to analyse the performance of the process. Thus, we have studied the power dissipation (in µW) in this process using COMSOL multiphysics software and the observed data is plotted using MATLAB. the graph is shown in Figure 6. The variation of power dissipation w.r.to excitation frequency shows almost same charecteristics as the variation of total energy w.r.to excitation frequency. The power dissipation is maximum (1.69 µW) at 105 Hz. The power dissipation is effectively high between 105 Hz - 110 Hz.

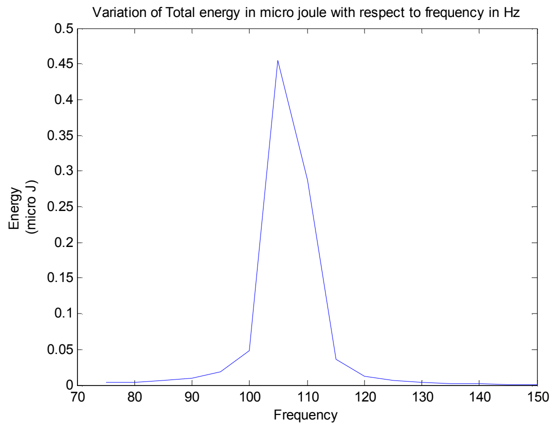

Figure 5. *Total harvested energy vs. excitation frequency.*

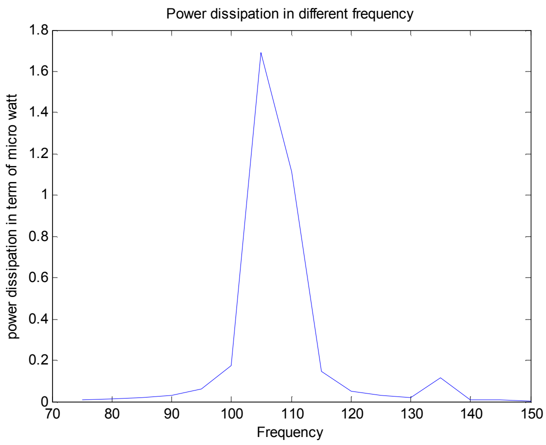

Figure 6. *Power dissipation during the harvesting of energy vs excitation frequency (piezoelectric material: Barium titanate).*

6.3. Variation of Potential Difference and Electric Power with Respect to Load Resistance

Load resistance is an important parameter to study the performance of Energy harvesting system using piezoelectric material. We have studied the variation of induced potential difference across the terminals of piezoelectric material (in volt) as well as the input mechanical power (in mW) and output electric power (in mW) with respect to load resistance at the resonant frequency 105 Hz. The graph is auto generated by the software, COMSOL multiphysics. The variation is shown in Figure 7. The peak of harvested energy from the device is in order of 10^3 ohm. The voltage becomes approximately constant above 10 KΩ. Initially, the input mechanical power is greater than output electrical power. But, the output electrical power becomes considerable higher than input mechanical power after 1 KΩ. The output electrical power as well as input mechanical power shows peak within the load resistance range 1 KΩ - 10 KΩ.

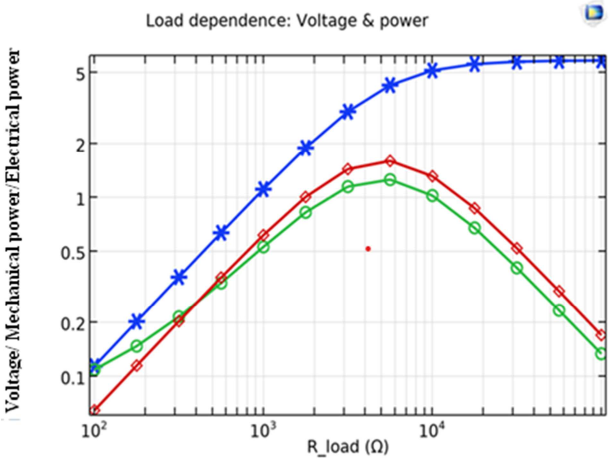

Figure 7. *The input mechanical power (in mW), the output harvested power (in mW) and the induced potential difference between terminals of piezoelectric material, Barium titanate (in volt) vs. load resistance (Ω).*

7. Conclusion

On the basis of above observations, it is concluded that the barium titanate gives very good response on frequency range 105Hz-110Hz and on load resistance range 1 KΩ - 10 KΩ.

Maximum voltage: 0.92068+2.3642i at 105Hz,

Max. Total Energy: 4.5438 X 10^{-7} J at 105Hz.

Thus the energy harvester works well on frequency range 105Hz-110 Hz. This model may be used in the railway track to harvest useful energy from useless rolling noise. This can solve the problem of energy crisis. The harvested energy can be stored in secondary cell for future use. The recharge facility of battery is independent of solar energy and other conventional energy. It depends on the rolling noise which is produced due to movement of Railway vehicle on the track. Additionally, this study can also be used to develop self-powered devices like Auto powered warning instruments.

The continuous research work for minimization of the energy loss is necessary. The future research is directed towards the development of the integrated form of transducer with power management and circuitry. This increases the generated power output from vibration (useless rolling noise).

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