Simulation and analysis of flexible TEG using polymer based and pyroelectric material for microdevice energy harvesting

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Abstract. Recently, an interest of thermoelectric generator (TEG) to manipulate and change heat waste into electrical energy has increased. The heat from electrical appliances, sun, human body, and natural environments can convert into electrical energy using TEG. However, typical conventional TEGs in the market have a hard and solid construction structure, hence difficult to bend according to curved surfaces of the heat sources. To overcome this problem, polymer-based material is proposing as the new packaging and substrate structure for the TEG. Besides, the thermoelectric conductor layer also changed using different types of pyroelectric for better heat absorption performance with low cost in mass-scale fabrication. Therefore, the simulation of eight pairs segmented conductive layer insulated with thin-film polymer due to standard modelling equation is present. The comparison of simulation with reference TEG to get the optimum output of temperature difference were also explaining. At the end of the simulation, polyimide as a packaging substrate with a conductive layer of Graphene (P-type legs) and Bismuth Telluride (N-type legs) has chosen for the best performance material for the flexible thermoelectric generator. The highest temperature difference produced by this design is 542°C for 0.945V input voltage and 120°C input temperature at the hot side.

1. Introduction

An increasing concern of environmental issues due to emissions especially in global warming and the limitation of energy resources has resulted a wide range of researcher to create new method and technologies including kinetic energy (wind, waves, vibration, gravity), electromagnetic energy (photovoltaic and radio frequency), thermal energy, hybrid energy and many more to generate electrical power [1,2,3]. Amongst there renewable method thermoelectric generation (TEG) has emerged as a promising new alternative energy technology in this few years [4].

TEG absorb waste-heat energy from certain sources, manipulate the energy using the Seebeck and the Peltier concept hence transforms into electrical power [3]. The thermoelectric generator is a solid-state technology, which allows direct conversion between thermal and electrical energy, with applications spanning from waste heat energy harvesting to precise climate conditioning. Conversely, in response to an input of electric power, the functionality is reverse and the same device is used for cooling [5]. TEG work upon applying a temperature gradient between the top and the bottom insulating layers thus current is generated and sustained.
The direct conversion of thermal energy into electrical energy provides a unique solution for continuous power to wearable devices. However, the inflexibility shape of conventional TEGs has resulted in a limit contact area of absorption with the thermal sources. This has significantly reduced heat recovery efficiency. There are varieties of flexible composite thermoelectric materials and devices developed previously based on conductive polymers, carbon-based materials, and inorganic nanomaterials [7-11]. Inkjet-printed using a large-area of flexible graphene film in excellent thermoelectric properties has reported [11]. Furthermore, most of the flexible substrates that used in wearable thermoelectric devices are polymer substrate materials based such as polydimethylsiloxane (PDMS), polyethylene terephthalate (PET), polyimide (PI) and many more [10].

In this paper, the previous TEG design is used as a reference to construct, simulate and analyse the performance of flexible TEG for thermal energy harvesting. The simulation and analysis of polymer-based material as the substrate layer and various kind of pyroelectric material as the thermoelectric element structure will vary with sort of parameter changes on these simulations and analysis. At the end of the investigation, the best material for the flexible thermoelectric fabrication will be chosen and proposed.

2. Design Structure

2.1. The design structure of a thermoelectric generator using polymer and pyroelectric materials

Figure 1 shows the reference structure of the TEG models. Eight thermoelectric couples (red and blue) are sandwiched between the aluminum nitride (AIN) plates (grey) and Cu electrodes (yellow). Two AIN plates are used as connection of couples because of its good thermal conductivity and electrical isolation. The size of the AIN plates is $25 \times 25 \times 1 \text{ mm}^3$. The thin Cu electrodes acting as wires are placed on one side of each plate. The size of the electrode is $3 \times 5 \times 0.03 \text{ mm}^3$ each. The other eight thermoelectric couples are sandwiched between the AIN plates and Cu electrodes with a size of $3 \times 3 \times 3.7 \text{ mm}^3$ for each thermoelectric legs. The n-type legs made from Bi$_2$Te$_3$ and PbSe$_{0.5}$Te$_{0.5}$, with a length of 2.0 mm and 1.7 mm respectively. The p-type legs consist of Bi$_{0.3}$Sb$_{1.7}$Te$_3$ segments and Zn$_4$Sb$_3$ segments, whose length is 1.7 mm and 2.0 mm, respectively [6, 8].

![Figure 1. The reference TEG structure with top plate hide](image-url)
2.2. The reference design of the thermoelectric generator

The design structure in this simulation are consisted with parameters of the substrate, thermoelectric legs, and copper electrodes and built according to the reference design [6, 8], but the type of materials for the substrate and thermoelectric materials were changed. In this simulation Polyimide (Pi) is used as the substrate and the thermoelectric structure materials for p-type and n-type legs were also substituted by using various types of pyroelectric materials varies from reference TEG, Bismuth Telluride (Bi$_2$Te$_3$), and Graphene. As illustrated in Figure 2, the substrate used is Polyimide (Pi) and the pyroelectric materials such as Graphene for P-type legs and Bismuth Telluride (Bi$_2$Te$_3$) for N-type legs.

![Figure 2. The designed TEG structure by using Pi, Graphene and Bi$_2$Te$_3$](image)

3. Simulation set-up

The flexible thermoelectric generator model is developed using COMSOL Multiphysics software to investigate and analyze the effect of parameter and material changing in determining the temperature differences and amount of electrical energy can generate.

3.1. COMSOL Multiphysics software approach

COMSOL Multiphysics is a simulation and development software to investigate and analyze the performance of flexible TEG structure in this study. First, the environment thus includes 3D dimensional geometry, thermoelectric physic, and stationery set-up. Then, the geometric objects were created by inserting the required parameters of TEG substrate, legs, and copper strips. The dimensions used in this TEG design is referred to as reference TEG in the previous research [6, 8]. Next, the parameters for each block were inserted by specifying the value of length, width and height in µm unit. After that, the properties of the materials for each of the TEG blocks are specified. For the built-in material, the material properties can be added to the TEG blocks. However, if the material is not available in the library, the material coefficient requires can be added manually into the table of material properties. Next, physical boundaries for each TEG block is defined. Meshing is the last process to do before run and simulation proceed. When there is an error detected, the boundary and parameter settings were check-up again. Otherwise, the simulation was run successfully, and the result can be analyzed to get an optimum output of temperature difference.

3.2. Basic circuit and formulation for the thermoelectric module

The generation of electricity from TEGs are depended on the Seebeck coefficient $\alpha$, while the Seebeck coefficient value depending on the semiconductor property. The voltage obtained from TEG can be calculated using the equation as follows:

$$V = \alpha \Delta T$$ (1)
where $\Delta T$ is the temperature difference between the TEG surfaces. From the equations, it shows that the voltage of TEG is directly proportional to Seebeck coefficient and temperature differences. Besides, the Seebeck coefficient is a constant value and can be clarified as below:

$$\alpha = \frac{2V_{\text{max}}}{\Delta T}$$

(2)

where the Seebeck coefficient is directly proportional with 2 times of $V_{\text{max}}$ and inverse proportional with the temperature difference between hot and cold as explained by the following equations as:

$$\Delta T = T_h - T_c$$

(3)

When there is no load connected at the end of TEG, the obtained voltage is known as the open-circuit voltage. When the pins of a TEG are short-circuited, the flowing current is called the short circuit current, $I_{\text{sc}}$. The maximum power derived from the TEG is a maximum value when the voltage of the open circuit and the current of the short circuit is half.

$$P_{\text{max}} = \frac{V_{\text{oc}}}{2} \times \frac{I_{\text{sc}}}{2}$$

(4)

$P_{\text{max}}$ quoted as the maximum power generated by the TEG. The figure of merit (FOM), $Z$ is a very crucial component in TEGs and given as,

$$Z = \frac{\alpha^2}{R_{\text{in}}K_{\text{th}}}$$

(5)

where, $R_{\text{in}}$ and $K_{\text{th}}$ are the internal resistance and the thermal conductivity of the TEG, respectively.

However, the internal resistance of the TEG, $R_{\text{in}}$ and the connected load resistance $R_l$ must match for an efficient conversion of the TEG. Therefore an internal rate and load resistance can be determined using,

$$m = \frac{R_l}{R_{\text{in}}}$$

(6)

The resistance rate is also taken into account while determining the for energy efficiency, current, and thermal conductivity. The thermal conductivity expressed as like:

$$K_{\text{th}} = \frac{\alpha^2}{R_{\text{in}}^2}$$

(7)

Depending on the resistance rate, the obtained current $I$ from the TEG given as follows:

$$I = \frac{a\Delta T}{(I+m)R_{\text{in}}}$$

(8)

TEG’s efficiency expressed in terms of both TEG properties and the input power of the system. It explained as follows, depending on the resistance rate.

$$\eta = \frac{mZ\Delta T}{(1+m)^2 + Z[(m+0.5)T_h + 0.5T_c]}$$

(9)
Moreover, depending on the system input power, $Q_h$, the TEG efficiency is represented as follow:

$$\eta = \frac{i^2 R_l}{Q_h}$$  \hspace{1cm} (10)

The maximum efficiency of TEG being not depending on the resistance rate clarified the following:

$$\eta_{max} = \frac{Z \Delta T}{4 + Z(1.5T_h + 0.5T_c)}$$  \hspace{1cm} (11)

If the efficiency value is known, the FOM value can also be calculated by the equation given below:

$$Z = \frac{4\eta_{max}}{\Delta T - \theta_{max}(1.5T_h + 0.5T_c)}$$  \hspace{1cm} (12)

From all the equations above, an assumption can be made that an efficiency of the TEG is highly dependent on the difference in temperature and load resistance in the circuit. The highest power results when load connected to the TEG output matches with the TEG’s material resistance.

4. Results and discussion

4.1. Results and analysis of TEG design using Polyimide and pyroelectric materials

Figure 3 shows the result of the output temperature difference produced by varying the types of material for the TEG design structure in this study. Based on the graph, its shown that temperature difference produces by reference TEG has the lowest output. When aluminium Nitride (AlN) plates substituted by Polyimide, the temperature difference increased by 45˚C. This is due to the excellent mechanical properties, high thermal and chemical stability properties of Polyimide. Instead of that, TEG that is made from Polyimide, Graphene and Bismuth Telluride. This is because Graphene is able to produce the highest temperature difference due to very high electrical conductivity. This result is aligned with the formula for the Figure of Merit, $ZT$ that stated the efficiency of a good thermoelectric material depends on the values of high electrical conductivity ($\sigma$), Seebeck coefficient ($S$), and low thermal conductivity ($k$) expressed as follows:

$$Z = \frac{S^2 \sigma T}{K}$$  \hspace{1cm} (13)

**Figure 3.** Temperature different against the type of materials
4.2. **Analysis of temperature different by varying the input temperature at the hot side.**

Figure 4 shows that there are not many changes in the output of the temperature difference produced by the TEG when the input temperature at the hot side are varied. Polyimide, Graphene and Bismuth Telluride materials show the highest temperature difference compared with the reference TEG. It is because the materials used has low electrical conductivity compared to other materials.

4.3. **Analysis of temperature different by varying the input voltage.**

In this simulation parameter of input voltage is vary from 20 to 120°C to analyze the output of temperature difference. Based on Figure 5, the temperature difference is directly increased proportionally with the increase of input voltage. Comparison has made from six materials chosen shown that the TEG built from Polyimide, Graphene and Bismuth Telluride has the highest temperature difference while the reference TEG obtained the lowest

![Figure 4. Temperature Difference against Input Temperature at the Hot Side Graph](image1)

![Figure 5. Temperature Difference against Input Voltage](image2)
4.4. Analysis of temperature difference by varying the dimension size

The simulation of AlN plates, Zn$_{0.5}$Sb$_1$, Bi$_{0.3}$Sb$_{1.7}$Te$_3$, PbSe$_{0.5}$Te$_{0.5}$ and Bi$_2$Te$_3$ design shown in Figure 6 used input voltage and input temperature of 0.945V at the hot side 120˚C. The maximum temperature produced is 231˚C, thus producing an output temperature difference of 111˚C. Although the dimension of TEG reduced from 25×25 mm$^2$ into 10×10 mm$^2$, the temperature difference still maintains the same result. Therefore, an assumption can be made that the dimension size does not affect the output temperature difference produced by the TEG.

![Figure 6. The simulation of 10×10mm$^2$ TEG structure](image)

5. Conclusion

Finally, the flexible thermoelectric using polymer and pyroelectric material has been constructed, simulated and analyzed. Besides, the performance of temperature difference with various parameter selection for the electrical generation was also investigated. Based on the analysis made up, the best design and material for flexible TEG structure propose is by using Polyimide as the substrate while Graphene (P-type legs) and Bismuth Telluride (N-type legs) as the thermoelectric element structure. Nevertheless, the design made up from Polyimide, Graphene and Bismuth Telluride materials has also given the highest temperature difference which entitles to produce highest electrical generation.

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