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Optimization of a Wearable Thermoelectric Generator Encapsulated in Polydimethylsiloxane (PDMS): A Numerical Modelling

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***Abstract*—To mitigate climate change attributed to the electricity generation, there have been tremendous efforts in replacing fossil fuels with renewable energies in the electricity sector. For this purpose, wearable thermoelectric generators (WTEGs) are the most promising direct and green power generation technique for portable electronics. In spite of extensive research, there is a trade-off relationship between the flexibility of WTEGs and their power output. Thus, this research aims to improve the performance of a flexible WTEG through differing thermal conditions around the hot and cold junctions. Accordingly, the PDMS substrate of a flexible WTEG is segmented into two layers, whereas each layer is individually filled with different fillers. Accordingly, three different patterns are proposed for the segmentation. Then, using COMSOL Multiphysics software, the output voltage and power of the specified patterns are analyzed and compared with those of an original flexible WTEG. Results concluded that releasing the thermoelectric legs from PDMS coating can remarkably improve the output voltage as well as the power generation. In addition, with regard to the segmentation pattern, adding fillers to the PDMS layers has a twofold effect on the voltage and power generation. Precisely, the thickness of each segment should be taken into consideration for selecting an appropriate filler. This work paves the way for enhancing the performance of flexible WTEGs, which ultimately leads to low carbon and energy-efficient electricity generation.**

Keywords-energy harvesting; additive; polydimethylsiloxane (PDMS); thermoelectric generator.

I. INTRODUCTION

Among the various renewable energy technologies, thermoelectric generators (TEGs) is a promising candidate for solving the energy problem from an environmental-sustainable viewpoint. Wearable TEGs utilizes the temperature difference between body skin and ambient to generate a low level of power current [1]. The amount of energy generated by a wearable TEG is in the range of ultra-low magnitude (nW) to middle magnitude (µW) [2]. However, there is an increasing need for more efficient TEGs to fit in with the recent advances in wearable electronics. Because of this, until to-date persistent efforts have been made to develop high-performance wearable TEGs. The primary approach to enhance the power generation of WTEGs is to employ thermoelectric legs and substrates (hot/cold) that possess respectively low and high thermal conductivities [3]. This is because, high thermal conductivity substrates accelerate heat dissipation at the interfaces (i.e. skin, TEG, ambient) [4]. In contrast, thermoelectric legs with low thermal conductivity decrease heat transfer across the legs [5]. Combining those, the temperature difference across the thermoelectric legs enhances, resulting in higher power generation.

In addition, it is desirable for a wearable TEG to be lightweight and flexible to avoid cumbersome for the users and to increase the contact area of the TEGs with curved surfaces of the body, such as wrist [6]. For example, in a conventional rigid TEG, see Fig. 1(a), thermoelectric legs are surrounded by air and sandwiched between two ceramic substrates. However, referring to the studies by [7-8], the flexibility of the conventional rigid TEG can be improved by removing the ceramic substrates and coating the thermoelectric legs and electrodes in a Polydimethylsiloxane (PDMS) substrate (see Fig. 1b). As can be seen, the ingot shape p- and n-type thermoelectric legs are connected with metallic interconnectors (copper) and enclosed in a stretchable elastomer (PDMS). Although coating the rigid thermoelectric legs in PDMS results in higher flexibility of the TEG compared to the conventional rigid ones, but it still suffers from lower power output.

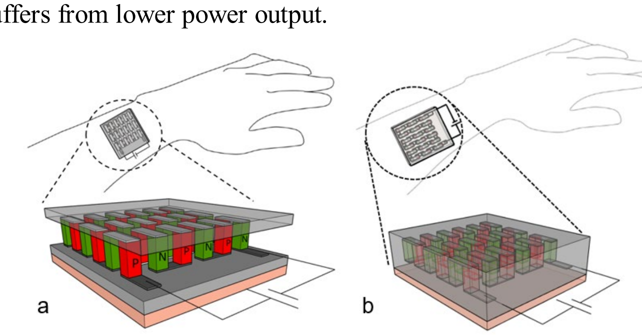

Figure 1. Schematics of a wearable TEG with 3D shape thermoelectric legs: (a) sandwiched between two rigid ceramic-based substrates; (b) encapsulated in a flexible polymer-based substrate.

In fact, there are two reasons for the lower power output of TEGs coated with PDMS compared to that of the conventional rigid counterparts. First, the thermal conductivity of PDMS (0.15-0.2 W/m.K [9]) is much lower than that of ceramic substrates (30-42 W/m.K [10]) in conventional rigid TEGs, which remarkably reduces heat transfer from skin to thermoelectric legs and from thermoelectric legs to air. Second, due to the higher thermal conductivity of PDMS than that of air, PDMS provides weaker thermal insulation around the thermoelectric legs compared to air (0.025 W/m.K [11]) in conventional rigid TEGs. As a result, although PDMS has the privilege of increasing flexibility of the TEGs, it provides a homogeneous thermal condition throughout the TEG, which deteriorates the power generation.

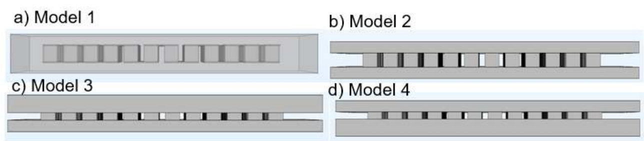

Figure 2. 3D configuration of the four specified models in COMSOL Multiphysics: (a) reference model; (b) PDMS covers the top and bottom electrodes; (c) PDMS covers the top half of the thermoelectric legs and bottom electrodes; (d) PDMS covers the bottom half of the thermoelectric legs and top electrodes.

Accordingly, this study aims to provide non-homogeneous thermal conditions across the flexible WTEG to enhance its power generation. To manipulate the thermal conductivity of PDMS, the common strategy is to incorporate fillers, including gallium-based liquid alloy [9], metals (Ag, Al, Cu, etc.) [12], and carbon-based materials, ceramics [12]. Accordingly, the single PDMS layer has been segmented into two PDMS layers, each covering either hot or cold junctions, and specific fillers have been added to each segment. As a result, the segmented PDMS substrate would provide different thermal conditions at hot and cold junctions due to different thermal conductivities of the fillers. Consequently, it is expected to enhance the power generation of the TEG by keeping one junction hot and the other cold. Therefore, there are two variables, which can be manipulated simultaneously to reach an optimum segmentation and an ultimate power output:

I. thickness of each segment
II. type of the added filler to each segment.

II. Methodology

In the present paper, computational modelling has been conducted using COMSOL Multiphysics to optimize the power generation of a TEG coated in PDMS with regard to variables I and II. Figure 2a shows the 3D model of a conventional flexible TEG, which is adopted as a reference model and contains a single homogeneous layer of PDMS substrate. The modelled thermoelectric legs representing the commercialized industrial Seebeck Effect Module GM 250-71-14-16 [13]. It has 72 pairs of rectangular-shaped P-type and N-type thermoelectric legs with 1.4mm width, 1.4 mm length and 1.6 mm height. The electrodes are 0.1mm thick. The thermoelectric legs are connected in series and thermally in parallel by the top and bottom copper strips. The dimension of the TEG is, 30 mm × 30 mm × 3.8 mm. To optimize the power output of Model 1 respecting variable I, the single PDMS layer has been divided into two layers. Fig. 2b-d illustrate three different segmentation patterns. As can be seen, the thickness and coating region of the PDMS layers vary in these three models. To manipulate the thermal property of the PDMS layers regarding variable II, three different fillers including air bubble, silver nanowire and gallium-based liquid alloy are individually added to each PDMS layers with a weight percent of 50 (wt%). Notably, configurations and properties of the thermocouple and interconnects is constant in the four models.

A. *Governing Equation*

The thermoelectric effect is the direct conversion of a temperature difference to potential difference and visa versa. The governing equations for determining the thermoelectric effect in the Joule heating equation are Maxwell and heat diffusion equations, which should be solved simultaneously:

Maxwell equation:

$$\nabla . J = 0 \tag{1}$$

$$E = -\nabla V \tag{2}$$

where J is current density (in A/m2), E is the electric field (in V/m) and V is electric potential (in V).

The time-varying heat diffusion equation:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla . q = Q \tag{3}$$

Here, ρ is the density of material (in kg/m3), C_p is heat capacity (in J/(kg K)), T is temperature (in K), q is energy density heat flux (in W/m2) and Q is the energy generation (in W). The related constitutive equations are:

$$q = -K\nabla T + PJ \tag{4}$$

$$J = -\sigma\,(E - S.\nabla V) \tag{5}$$

$$Q = J.E \tag{6}$$

where P is Peltier coefficient (in W/A), S stands for Seebeck coefficient (in V/K), and k stands for thermal conductivity (in W/mK). In this work, since heat diffusion is determined to be constant, Equation 3 can be simplified as:

$$\nabla q = Q \tag{7}$$

B. *Boundary Conditions*

Fig. 3 indicates the boundary conditions of Model 1, which is consistent in the other three models. Accordingly, the following assumptions are made:

- To simplify the simulation, the thermal conductivity, Seebeck coefficient, and electrical conductivity are temperature independent.

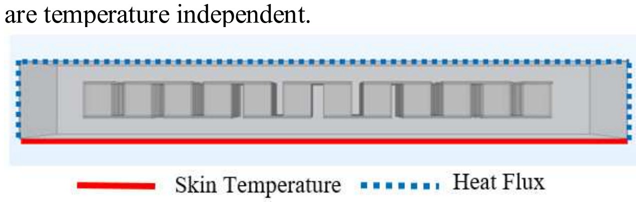

Figure 3. An illustration of the defined boundary conditions in the COMSOL Muliphysics

- A constant temperature (T_{hot}) of 24°C is applied to the bottom surface of the PDMS substrate, which is equivalent to the skin temperature.

- The initial temperature of the TEG is 15°C, which is equal to the defined outdoor temperature (T_{cold}).

- In order to study the electric potential, one side of the last n-type leg is grounded (V=0) assuming that the potential current flows from the p-type leg towards the n-type leg.

- No external electric potential passes through the module.

C. *Material Properties*

Thermoelectric materials are characterized by three parameters including Seebeck coefficient, electrical and thermal conductivities. Most contemporary TE devices use bismuth telluride as a thermoelectric material. Therefore, it can be assumed that both n-type and p-type legs are composed of properly synthesized Bi_2Te_3. Therefore, the formulas and data provided in [13] have been chosen to approximate the thermal conductivity λ, Seebeck coefficient α, and electrical conductivity σ of n-type and p-type semiconductors. Table 1 summarizes some properties of the materials used in the simulation. Results.

TABLE I: THE PROPERTIES OF MATERIALS EMPLOYED IN THE SIMULATION

	Thermal conductivity [W/m.K]	*Electrical conductivity [S/m]*	*Seebeck coefficient [V/K]*	*Density [kg/m3]*
p-Bi2Te3	1.65	$1.27e^{6}$	$1.89e^{-4}$	7700
n-Bi2Te3	1.67	$1.08e^{6}$	$-2.1e^{-4}$	7700
PDMS	0.15	10e-14	-	965
Air	0.02	0	-	1.2
Silver Nanowire	180	-	-	779
Galinstan	16.5	3.3e6	-	6440

D. *Voltage Output*

Fig. 4 indicates the open-circuit voltage of the 16 specified samples. It should be noted that T and B denote Top and Bottom layers respectively. Therefore, T-air/B-air refers to the samples composed of air bubbles as an additive both in the top and bottom layers. As it can be seen, model 1, which contains a single PDMS layer, obtains the lowest voltage both with and without adding fillers. However, segmenting the PDMS substrate (models 2 to 4) remarkably improves the output voltage of the TEG compared to that of model 1 even without adding any fillers. In particular, the maximum output voltage of 10mV has been achieved by model 2, which its PDMS layers only covers the electrodes, but not the thermoelectric legs. The primary reason is that air contains lower thermal conductivity compared to PDMS, thus model 2 provides superior insulation around the thermoelectric legs compared with models 3 and 4. It is exactly the same rule when the voltage output of model 2 falls due to adding air bubbles to the top and bottom layers. Conversely, a maximum voltage of model 2 is achieved by adding high thermal conductivity fillers, including Galinstan and silver nanowires, to both layers.

In addition, Fig. 4 indicates the converse effect of similar fillers on the voltage output of models 3 and 4. To illustrate, although adding high thermal conductivity fillers to the bottom layer of model 3 leads to the highest values, but it results in the lowest output voltages in model 4. The main reason is that adding a high thermal conductivity filler to the bottom layer of model 3 can compensate its lower thickness compared to that of model 4. Whereas, adding the same filler to the bottom layer of model 4, intensifies heat accumulation in the hot junctions, resulting in faster heat transfer across the thermoelectric legs and ultimately lower output voltage. The same is true for the top layers of models 3 and 4. Therefore, concerning maximum output voltage, there is a converse relationship between the thickness of the layers and thermal conductivity of the fillers.

E. *Power Output*

Regarding Fig. 5, improving the power output of the reference model is not necessarily dependent on adding a filler. To put it another way, even segmenting the pristine PDMA substrate into two layers can improve the power output up to 5 to 6.5 order of magnitude. This is because, in

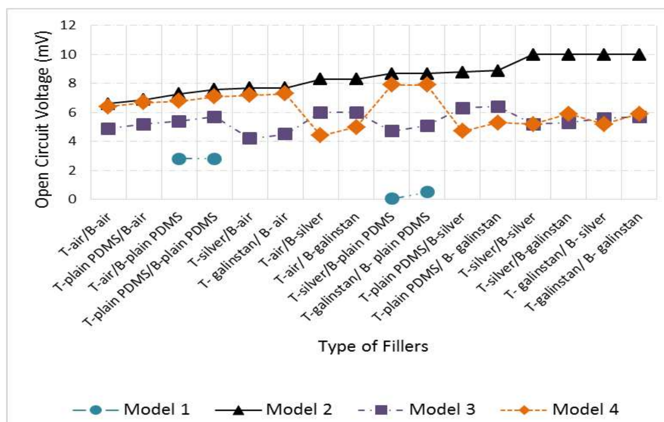

Figure 4. Comparison between the generated output voltage of the four models, when different fillers are added to their substrates.

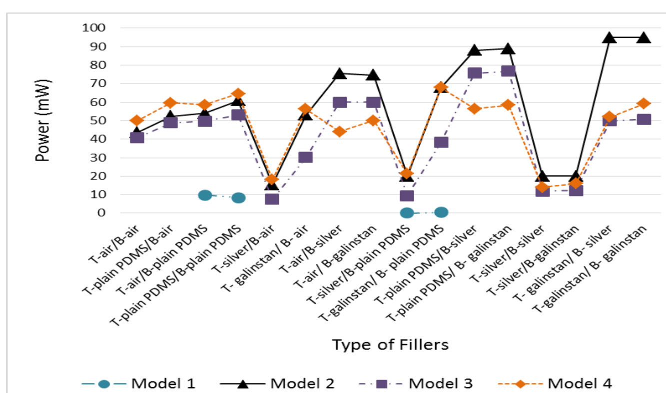

Figure 5. Comparison between the generated power output of the four models, when different fillers are added to their substrates.

the defined segmented models (2 to 4), the thermoelectric legs come in contact with air instead of PDMS. Therefore, the notable lower thermal conductivity of air compared with that of PDMS increases the temperature difference across the legs. However, adding silver nanowires to the top layer of models 2 to 4 is the worst-case scenario, which can even lead to a power output lower than that of the reference model. It could be interpreted by the remarkable reduction in the open circuit current in these models owing to adding silver nanowires to the top layer. Concerning model 2, using a high thermal conductivity filler in the bottom substrate enhances the power output. Besides, this improvement could be further enhanced by adding a high thermal conductivity filler to the top layer as well. Therefore, model 2 with top and bottom layers filled with Galinstan obtains the optimal power value of 95mW. Evaluating the impact of layers' thickness on fillers' selection, it should be noted that model 3 is superior to model 4 when their top and bottom layers are filled with low and high thermal conductivity fillers, respectively. Conversely, for model 4, fillers with high and low thermal conductivities are suitable for the top and bottom layers, respectively.

III. Conclusion

This work investigated the potential of segmenting the PDMS substrate of a WTEG and adding fillers to the segments to generate higher electricity. Based on the 3D model simulations the relationship between the thermal properties of the fillers and thickness of the segments has been studied, resulting in the following conclusions.

(1) Adding a high thermal conductivity filler to the reference model deteriorates the power and voltage generation. Therefore, it is strongly recommended to either keep the PDMS substrate of the reference model pristine or add a low thermal conductivity additive to it.

(2) When no filler is added to the PDMS substrate, the most striking strategy is covering the bottom half of the thermoelectric legs with PDMS and keeping the top half exposed to air. This approach can improve the power output of the TEG up to 6.5 order of magnitude.

(3) The maximum power output could be achieved when only the electrodes are covered by the PDMS substrate, but not the thermoelectric legs. To illustrate, the difference between the highest power output obtained by model 2 and that of models 1, 3, and 4 are 85mW, 15mW and 25mW respectively.

(4) Finally, comparing models 3 and 4, fillers should be determined with respect to the layers' thickness. Precisely, the thicker the layers are, the lower thermal conductivity the fillers should have and vice versa.

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