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Geometrical optimization of a thermoelectric device: Numerical simulations

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ABSTRACT

In the present work, through the use of the COMSOL Multiphysics software, thermocouples (TCs), constituted by a p and a n type leg, and thermoelectric (TE) devices with different geometries are numerically simulated aiming for an optimized geometry. The semiconductor material used in the simulation is bismuth telluride (Bi_2Te_3) and copper (Cu) is used to achieve the electrical contact between the TE pillars. Two geometries of the thermocouple legs are studied, cubic and cylindrical geometries, revealing that both present identical performances under the same conditions. From these simulations, the optimal ratios achieved between the various geometrical parameters of the TC's are analysed. It was verified that it exists an optimal ratio between the height and the width of the TE legs with the value 5×10^{-3}. Moreover, it is shown that increasing the cross-section area of the legs enhances the power produced by a TC. It was also observed that the length of the copper contacts should be smaller than 0.05 times the width of the TE legs for the best performance to be achieved. It was also established that there is an optimal ratio between the copper contacts height and the TE legs height, being, approximately, 40. For a TE device, an increase in the number of TC's is favourable towards a better performance.

1. Introduction

The paradigm of world energy consumption is a concern that must be addressed in the near future. There is a demand for the use of new sources of energy, namely generation of sustainable energy using efficient methods. This paradigm leads to the concept of energy harvesting or energy scavenging which is gaining more importance in the last years [1,2]. Several technologies of energy recovering with promising outputs already exist. These use mechanical movement, pressure or temperature [2]. Taking advantage of mechanical movements or pressure, Triboelectric and Piezoelectric generators are extensively studied in parallel to Magnetic Induction based devices [1,3]. Triboelectric generators were invented as new way of harvesting energy using the coupling of the triboelectric and electrostatic effects. Recently, nanostructures have been used, which increases the efficiency up to 100%, making Triboelectric generators the technology with the most prominent growth [4]. Other technologies that use movements or pressure (i.e. Piezoelectric and Magnetic Induction), in spite of, nowadays also being at the nanoscale, did not achieve outputs like Triboelectrics [1–3]. On the other end, Photovoltaic panels and Biomass are technologies already present in the market.

All these technologies are being developed or effectively applied, using energy that otherwise would go to waste. However, heat is still the form of energy that is widely wasted. The thermoelectric effect is the unique phenomena that can directly convert waste heat into electrical energy and vice versa. It is based on the Seebeck effect which is the generation of electricity due to a temperature difference. This effect is the basis of TE generators [5,6]. Although there is an enormous amount of waste heat all around us (home heating, cars, industries…), these generators are not yet widely used because their efficiency is not sufficient to attend our world's demands. Therefore, there is a need of enhancing the performance of TE generators [5–7].

A typical TE device contains a certain number of thermocouples (TCs) that are made of p-type and n-type semiconductor legs (the TE material) connected electrically in series and thermally in parallel. A temperature difference is imposed between the top and bottom of the legs and an electrical voltage is generated [5]. Until now, the creation of complex TE materials with enhanced figures of merit or the improvement of the fabricated TE devices are the main efforts for the advance of TE generators. For example, Ref. [6] is a review of the working principle of a TE generator and coolers, where an overview of the current research into TE materials is also given. These materials can be characterised into three categories such as semiconductors, ceramics (metallic oxides) and polymers (carbon nanotubes in polymer-matrixes). On Ref. [7], the material's transport properties that influence the efficiency of a TE material are explained and several complex TE materials being developed nowadays are discussed. These materials are, for example, alloys of Bi, Te and Sb as well as skutterudite alloys like $CoSb_3$.

Another way to optimize TE devices is to perform numerical

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simulations. So far, these simulations focus either on optimizing a certain material property or on studying a type of device under a set of experimental conditions, to draw a comparison between the theoretical behaviour and the experimental results. One example of these type of TE generators development is the work of Refs. [8,9]. As a first part of this work, they used commercially available TE generators to realise experimentally a heat exchanger based on cold and hot fluid flows. On the second part of their work, they simulated using finite element methods their TE generator based heat exchanger, in order to have a comparison between the experimental results they obtained and the theoretical expected behaviour. Refs. [10,11] are also two examples of simulations of TE generators being used to have a greater insight into a certain application of the generators or for a comparison with experimental results. The COMSOL Multiphysics software has been widely used in simulations of the TE effect. The previously referred work [9] was performed using COMSOL Multiphysics, as well as Ref. [12], where the numerical simulations where conducted to have a comparison with the experimental results of a TE generator. However, simulations performed using this software focus on studying only a certain novel device. Studies of the geometry of TE devices using simulations are still ongoing. On Ref. [13], the authors simulate two types of devices with distinct TC's and study how their efficiency depends on the width of the legs and number of these TC's. However, their main focus was also the simulation of the heat source and a comparison and validation of the numerical results with the experimental studies. There is still a lack of systematic geometrical studies of a TE device, with not only a focus on the geometry of the TE material but also on the electrical contacts geometry. Thus, the aim of this work is to numerically simulate the influence of the geometric parameters of the TE material and of the electrical contacts towards the optimization of the TE device. The optimization was made in three phases: (i) the study of the geometry of the TE legs of a TC; (ii) the temperature dependence of the power output, (iii) the study of the geometry of the electrical contacts and (iv) the study of the optimal number of TCs on a TE device. These studies were made by numerical simulations performed using the COMSOL Multiphysics software.

2. Numerical considerations

The 3D geometries studied and their materials are represented in Fig. 1. For the numerical simulation, it was considered that both geometries are constituted by two legs of a material with physical properties similar to bismuth telluride (Bi_2Te_3) with their difference being the signal of the Seebeck coefficient, allowing one leg to be considered as a p-type material and the other n-type. Moreover, to insure the electrical contact between the legs, three layers of copper (Cu) were also included. Insulating layers as in classical TE generators were not included due to the performed studies being the ideal behaviour, without heat losses. The geometrical parameters of the legs were height (H) and width (L) for the square geometry whereas for the cylindrical geometry it was considered radii (R). In both geometries, the copper contacts have a height (h) and length (D) when connecting the TE legs, with the bottom ones having the same base as the legs and the one at the top achieving the electrical contact between the two TE legs. The TE device is constituted by a certain number of TCs as the ones described, with a p-type leg connected to two n-type legs by layers of copper, as represented in Fig. 2.

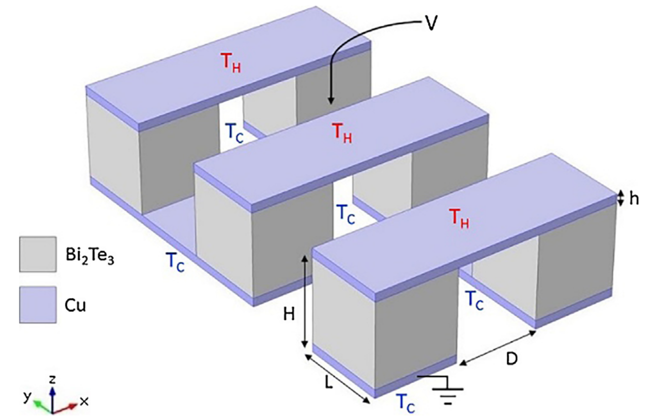

Fig. 2. Schematic geometry of the thermoelectric device considered with cubic thermocouples and boundary conditions.

The COMSOL Multiphysics 4.4 was the software used to perform the simulations. The TE module inside the heat conduction module was the basis for all the simulations. This module uses finite element methods (FEM) to solve the equations that describe the TE effect: the heat conduction equation in solids and the continuity of electric charge equation with the constitutive TE equations [14–16]. FEM is a numerical method in which the system is divided into smaller systems (finite elements) where the simpler equations that govern each of the finite elements are assembled into a large system of equations, which are then solved using variational methods to minimise the associated error function. The studies carried out are stationary and without a magnetic field. Considering this, the system of coupled TE equations that the module solves is:

$$\begin{cases} -\nabla((\sigma S^2 T + k)\nabla T) - \nabla(\sigma S T \nabla V) = \sigma((\nabla V)^2 + S\nabla T \nabla V) \\ \nabla(\sigma \nabla V) + \nabla(\sigma S \nabla \boldsymbol{T}) = 0 \end{cases} \quad (1)$$

where T, V, S, k and σ are the absolute temperature, the electrical potential, the Seebeck coefficient, the thermal conductivity and the electrical conductivity, respectively [14,17].

For the TE module to solve the system of equations, two different

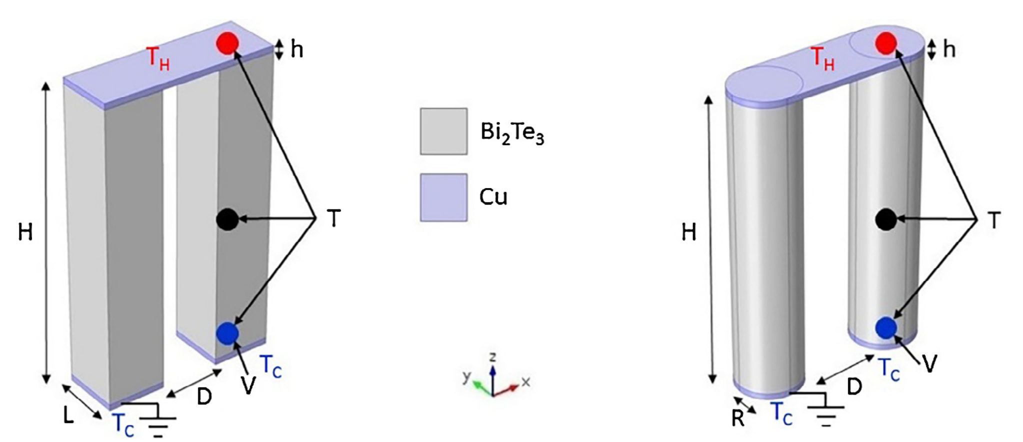

Fig. 1. Schematic geometries of the thermocouples considered: cubic and cylindrical, and boundary conditions.

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