Foundational undergraduate teaching and research tools in thermoelectrics using Comsol Multiphysics

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Introduction

Comsol Multiphysics can play a crucial role in jumpstarting undergraduate research programs in physics and engineering at colleges with limited financial support and small faculty size. The engineering physics program at Ramapo College of NJ has 48 majors and 4 full time faculty with full teaching responsibility, limited research time and financial resources. An attractive experimental and Comsol Multiphysics project based on physics topics covered in the curriculum can lead to a rewarding experience for both the students and faculty. One example is the thermoelectric generator. Due to increasing global demand for energy, climate change and a need for sustainable energy solution, thermoelectric generators are considered a very appealing clean option. Despite their relatively low efficiency, recent developments in nanotechnology prove that their response can be improved and therefore a resurgence of research projects are dedicated to increasing their thermopower while reducing the thermal conductivity and increasing the electric conductivity of the electrical contacts. The current project presents a three-component model of a commercial thermoelectric generator with water, heat sink and air-cooling. The electric potential induced by the Seebeck effect was computed for common and novel materials as a function of the temperature of the cold and hot surface temperature and the cooling water. An optimized set of TEG parameters for a practical application is sought. The work presented is the first step in the development of an undergraduate materials science laboratory. It is also used to develop teaching apps for the engineering physics curriculum and to develop Comsol Multiphysics modeling skills for faculty and students.

Theory / Experimental Set-up

The thermoelectric (TE) effect was discovered and studied by the German scientist Thomas Johann Seebeck beginning with 1821. Seebeck discovered that two different materials with junctions held at different temperatures deflect a compass needle. Due to the temperature difference, a current is produced. According to Ampere's law, the current produces a magnetic field, which in turn will deflect a magnet. The voltage produced is proportional to the temperature difference between the "hot" and "cold" contacts and independent of the distribution of temperature along the materials. The proportionality constant is the Seebeck constant S, a primary characteristic of TE materials. This phenomenon is the basis of thermocouples. The reverse is also true. In 1834, the French scientist Jean Charles Athanase Peltier found that a voltage difference applied to a junction of two different TE materials leads to a temperature difference (the Peltier effect), currently used in Peltier coolers. The proportionality constant P, is called the Peltier constant. Neither scientist gave a theoretical explanation of the phenomena. In 1854, Lord Kelvin (formerly William Thomson) explained the phenomena and the relationship between the coefficients using principles of the thermodynamics and in the process predicted the third thermoelectric effect, the Thomson effect. Briefly, when a temperature gradient is applied to a TE material, a current will flow through the material leading to heat absorption or emission (1). The amount of heat is proportional to the current as well as the temperature difference through a constant called the Thomson constant. Based on the work of Edmund Altenkirch and Abraham Fedorovich Ioffe, a parameter called "figure of merit" zT, was introduced in in 1956 in order to characterize the performance of a thermoelectric device. In 1954 H. Julian Goldsmid introduced the concept called thermoelectric quality factor in order to characterize the efficiency of semiconductors. While heavily studied and developed in the former USSR in the midlle of the 20th century, thermoelectric have undergone cycles of high and low interest. The advancement of nanomaterials fabrication in the early 1990s renewed

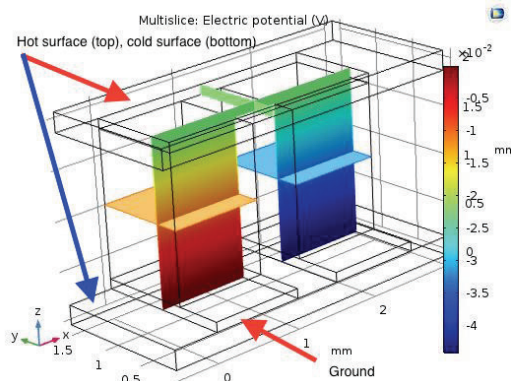the interest in TE materials as it was shown that the zT can be increased well above 1.

Fig. 1 The Seebeck effect in a pair of Bi_2Te_3 with Cu contacts.

A thermoelectric generators is made of three basic components: an array of thermoelectric material with a simple rectangular box leg, electrical contacts to connect the legs in series or parallel and two parallel isolating plates that sandwich the other two components. Two electrical wires conduct the electrical current to the external load.
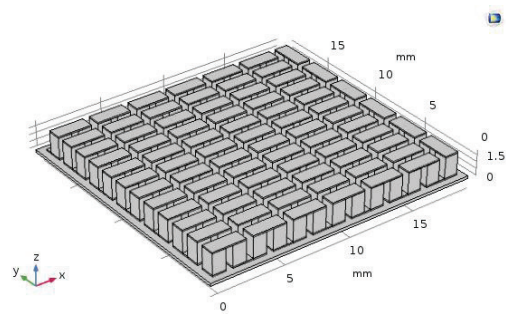

Fig. 2 A simplified schematic for a commercial TEG in series connection (drawn here without the top insulating alumina face).

The performance of thermoelectric generators depends on the zT value of the material used which in turn depends on the hot face temperature and temperature differential between the plates (3). The temperature dependence can be improved by segmenting the legs, which means fabricating each leg by stacking vertically two different thermoelectric materials where each segment performs better for the temperature range expected along that particular segment (4). While the overall thermoelectric efficiency of the segmented leg could be superior to the non-segmented approach, the contact surface between the two materials introduces additional electrical contact resistance which lowers the leg

efficiency. Several methods of optimizing the thermoelectric efficiency by analyzing the effects of the contact thermal and electrical resistance have been discussed (4, 5). Another way to increase the thermoelectic efficiency is to increase the value of the Seebeck coefficient by changing the way they are fabricated. W. Li et al developed thin films of n-type and p-type thermoelectric materials and have shown increased Seebeck coefficients and power factors (7). Other groups developed complex thermoelectric materials with high zT such as skutterudites and Zintl phases by using novel technologies in nanostructural engineering (1). Other have developed high zT materials by incorporating a matrix of nano-particles (8-16), single or multi-wall carbon nano-tubes (17) or graphene (20). Finally, a most exciting development in photonic topology showed that new thermal metamaterials can control the emission of a hot object by enhancing a certain portion of the spectrum and reducing the rest (21). With such material interfaces the spectrum emitted by a hot surface can be tailored to the match the energy gap of the thermoelectric material therefore promoting more charge carriers to the conduction band and reducing heat waste. The efficiency of a TEG can also be significantly improved by adding a cooling system that carries away heat from the cold and therefore keeps the cold face at a lower temperature for longer periods of time. In addition to a fluid cooler, a heat sink offers additional cooling and a combination of both is often employed when commercial TEGs are developed. Various versions of these systems have been commercially developed for car engines, outdoor activities as well as space missions (1).

In a dual-stage microthermoelectric generator study it was shown that the area over the length of the thermoelectric leg plays a role in the overall performance and it is maximum at a value of 0.78 at a temperature difference of 20deg C (5). Another study (6) measured the independent effects of leg area and length over a wider range of temperatures with including water and heat sink cooling and found no effect of the leg surface area. However, their study shows that increasing the leg height significantly improves the electrical performance while having no significant effect on the thermal performance.
Novel nanoengineered materials (8-17) show remarkable thermoelectric properties such as high Seebeck coefficients and ZT values. Other nanoengineered materials prove to be excellent electrical contact materials (18-20) with physical characteristics competing with Cu. Several groups have developed industrial applications of TEGs for commercial purposes such as car engines or buildings (22-25).

The work presented here is a preliminary study of the materials and configurations that could lead to a more efficient TEG prototype. This project was conducted by a group of undergraduate engineering physics majors under supervision. Specifically, we have completed the following:

A. Develop a Comsol stationary model for a square array of N pairs of thermoelectric n- and p-type materials that mimic TEG elements available commercially (tegpro.com) Ad a water cooler and a heat sink to the cold side of the TEG in order to extract the heat. Investigate the efficiency of the TEG for various hot surface and inlet water temperatures

B. Research the literature for new high ZT thermoelectric materials, compile a table of thermoelectric constants and calculate theoretical values when experimental values are not available using the Kopp-Neuman rule

C. Run the program for the novel thermoelectric material (nanostructured BiSbTe) and compare the electric potential against two common thermoelectrics, Bi_2Te_3 and PbTe. To the best of our knowledge there is no Comsol thermoelectric data reported on BiSbTe

Work in progress includes:

D. Research and compile a list of new nanostructured materials that could substitute Cu as the electric contact materials used today and generate improved performance and/or reduced cost

E. Investigate various water cooler geometries, water injection conditions and materials for increased TEG efficiency

F. Investigate various heat sink geometries and materials for increased TEG efficiency

G. Test the theoretical Kopp-Neuman heat capacity values against experimental values for nanostructured materials fabricated in the materials science lab

Experimental Set-up

The model proposed is a replica of a 5cmx5cm commercial TEG module (tegpro.com) with 1mmx1mmx1.5mm (WxDxH) thermoelectric blocks connected in series. The electric contacts are 1.5mmx1mmx0.1mm. The blocks and contacts are sandwiched between two alumina sheets, 50mmx50mmx1mm. A water cooler with an inlet and outlet (tegpro.com) is sandwiched between the TEG and an aluminum heatsink. The system is enclosed in a rectangular box to allow for convection cooling by

air. The computer model was compared to the standard Bi_2Te_3 commercial module for a variety of hot temperature values (Fig. 3). The water cooler was fed by a sink with the temperature of the inlet T_{inlet} = 19degC. The experimental data was collected with and without airflow produced by a fan. The experimental data (voltage versus time) was collected with Vernier LoggerPro software. Without cooling the commercial module produces a low voltage (just over 0.2V) that drops as the temperature difference drops. At temperatures higher than 160C the module is easily destroyed if cooling with water or air is not provided. Fig. 3 below shows the dependence of the voltage on the fan speed. The TEG is water cooled for the first 2300s. At that time, the fan is turned on. As the fan speed is increased from level 1 to 2 and 3, the graph shows the voltage increasing in three stages.
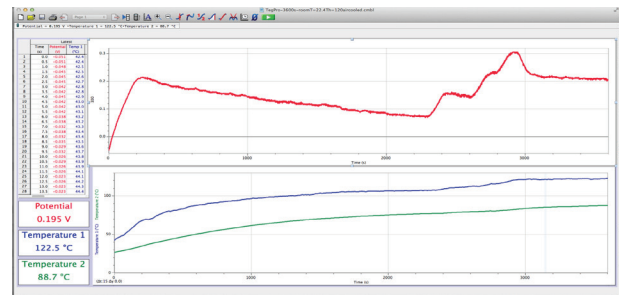

Fig. 3 Experimental data on a commercial (2) TEG module with water cooling at 19C, T_{hot} = 162C and T_{cold} room temperature T_{cold}=22C, with the fan off and on.

Our simple experiment clearly shows the effect of the air cooling and the water cooling on the TEG performance. The model we propose seeks to increase the TEG efficiency in the range of common applications at reasonably looking at several factors:

a. thermoelectric material
b. electric contact materials
c. water coolers
d. convection cooling with air

Governing Equations / Numerical Model / Simulation / Methods / Use of Simulation Apps

The program uses the Heat Transfer Module for a stationary study. We coupled the Laminar Flow and Heat Transfer interfaces by adding a "Nonisothermal Flow" Multiphysics node and included the Thermoelectric effect. The equations describing the heat transfer by conduction and convective cooling, the electric currents and the Joule coupling, as well as the thermoelectric effect are fully described in reference (27) which was used

as an example to develop the thermoelectric calculations. The program solves for heat transfer by conduction at all interfaces and water convection.
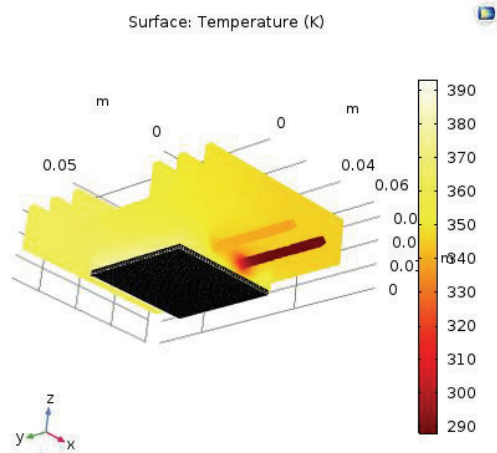

Fig. 4 Temperature graph for the complete 3-component model with TEg module, water cooler and heat sink.
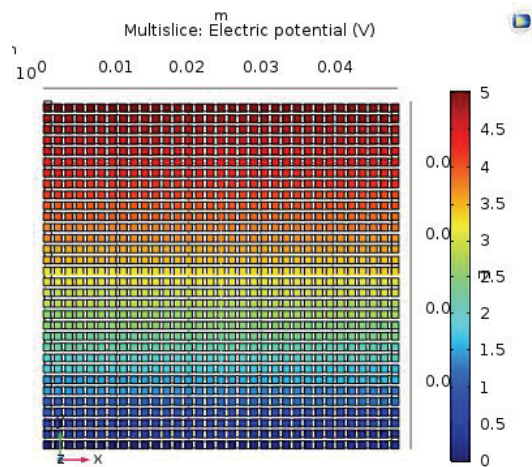

Fig. 5 Electric potential for a TEG with water cooler and heat sink with T_{cold} = 293K and T_{hot} = 393K. T_{inlet} water = 291K

The Solver was configured for the Automatic(Newton) method which significantly reduced the computation time. The materials physical constants were taken from Comsol Materials database for Bi2Te and PbTe. New materials with physical properties found in literature and/or theoretically estimated were added. The program does a parametric sweep over temperature, thermoelectric leg height and inlet water temperature and a material sweep over the materials to be tested. The bottom surface of the TEG at in contact with the hot surface. The entire system starts at room temperature. Several apps have been developed for parts of the program with the goal of

using them as lecture or research tools. Such examples are: the two-leg pair in the Seebeck and Peltier mode, a full model of the commercial TEGPRO modules, water coolers of different materials and geometries (in progress), heat sinks of different materials and geometries. More small teaching programs are in progress.

Experimental Results / Simulation Results / Discussion

The first data set obtained is the electric potential generated as a function of the hot surface temperature for four thermoelectric materials, Bi_2Te_3, PbTe , Spark Plasma Sintered Cu_2Te and nanostructured BiSbTe. The test model is composed of just a set of three semiconductor pairs connected in series, with no external cooling. The cold face temperature is maintained at 293.15K. Fig. 6 summarizes the electric potential generated for a range of temperatures. Bi_2Te_3 is clearly the best thermoelectric material in this group, in good agreement with published experimental measurements of thermoelectric properties for the range of temperatures below 550K (2).
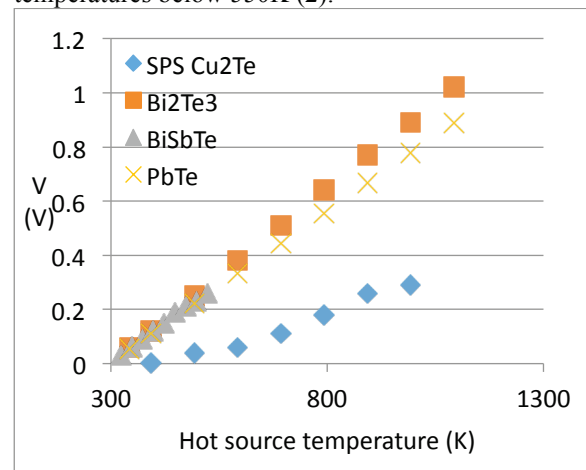

Fig. 6 Electric potential generated by four thermoelectric materials (three semiconductor pairs in series) as a function of the hot source temperature.

Fig. 7 shows the electric potential for the same materials but for the full TEG module with both water and heat sink cooling. The cold water inlet is maintained at 288.15K. An interesting change in performance takes place when cooling is added. At T=390K, BiSbTe generates an electric potential 23% higher than Bi_2Te_3.
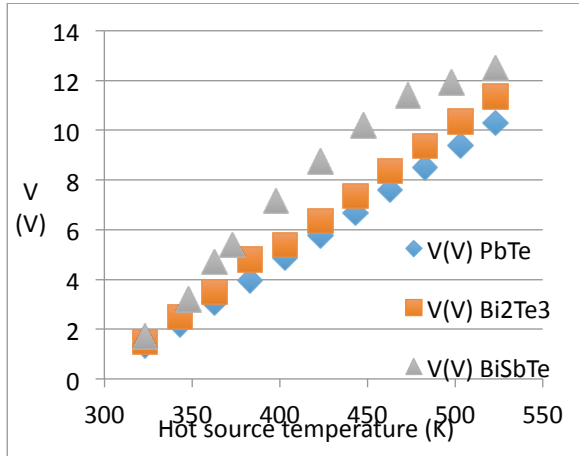
Fig. 7 Electric potential induced via thermoelectric effect as a function of hot surface temperature for three thermoelectric materials. Data shown for a full size module with water and heat sink cooling.

The temperature of the outlet water for different thermoelectric materials as a function of the hot surface temperature is shown below. Bi_2Te_3 and PbTe are the best at transferring the heat to the water most likely due to the values of thermal conductivity which decrease from Bi_2Te_3 to PbTe to BiSbTe (28).
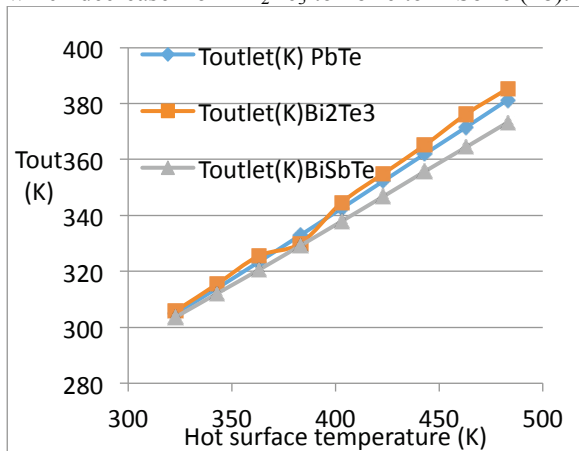

Fig. 8 Outlet water temperature for different thermoelectric materials as a function of the hot surface temperature.

It has to be emphasized that the results of a computer model are meaningful only if the physical constants entered in the model are correctly selected and if the materials are compared for the same temperatures. As an example, we used the spark plasma sintered Cu_2Te physical constants (thermal conductivity, electric conductivity, heat capacity at constant pressure and Seebeck coefficient) measured at 400K and generated a set of data for a temperature range between 393K and 1093K The model had only three pairs of semiconductor blocks with no water or heat sink.

Next, we extracted these values for eight temperature points starting at 393K up to 1093K in equal steps of 100K (16) and repeated the calculations one set of values at a time. The results for both scenarios are summarized in Fig. 9. At 893K the calculated electric potential is 60% higher than the one calculated for the same temperature but with physical constants measured at a different temperature. Therefore, while researching materials and their physical constant values for new thermoelectric efficient materials, extreme care needs to be taken in extracting them from published data or measuring the values of these constants as a function of temperature.
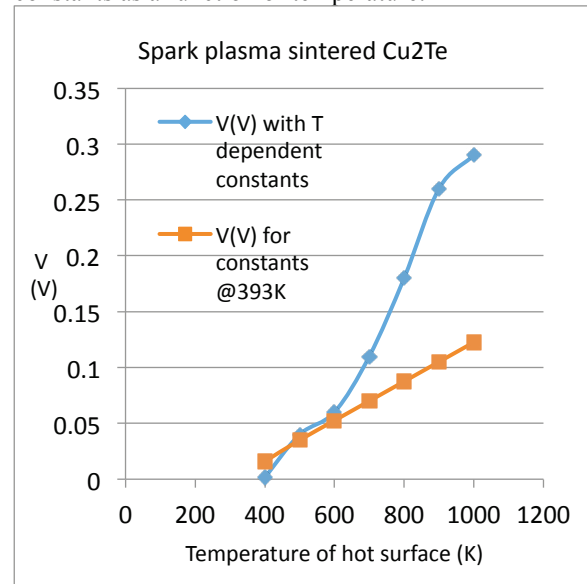

Fig. 9 Electric potential for a SPS Cu_2Te TEG model calculated using a set of physical constants measured at 393K and measured at each temperature value used in the simulation.

Conclusions

Comsol Multiphysics played a significant role in spurring interest and ideas for an undergraduate materials science laboratory that combines fabrication, characterization and modeling. Several applications have been developed and incorporated in the engineering physics curriculum and several students are being trained in developing applications with Comsol. Nanostructured BiSbTe proves to be a superior novel thermoelectric under water cooling conditions. The computer simulations demanded material properties research which in turn suggest fabrication and characterization ideas for the new materials science laboratory at Ramapo College of NJ.

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