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Three Dimensional TCAD Simulation of a Thermoelectric Module Suitable for Use in a Thermoelectric Energy Harvesting System

Chris Gould and Noel Shammass

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1. Introduction

Thermoelectric technology can be used to generate electrical power from heat, temperature differences and temperature gradients, and is ideally suited to generate low levels of electrical power in energy harvesting systems. This chapter aims to describe the main elements of a thermoelectric energy harvesting system, highlighting the limitations in performance of current thermoelectric generators, and how these problems can be overcome by using external electronic components and circuitry, in order to produce a thermoelectric energy harvesting system that is capable of providing sufficient electrical power to operate other low power electronic systems, electronic sensors, microcontrollers, and replace or recharge batteries in several applications. The chapter then discusses a novel approach to improving the thermoelectric properties and efficiency of thermoelectric generators, by creating a 3D simulation model of a three couple thermoelectric module, using the Synopsys Technology Computer Aided Design (TCAD) semiconductor simulation software package. Existing published work in the area of thermoelectric module modelling and simulation has emphasised the use of ANSYS, COMSOL and Spice compatible software. The motivation of this work is to use the TCAD semiconductor simulation environment in order to conduct a more detailed thermal and electrical simulation of a thermoelectric module, than has previously been published using computer based simulation software packages. The successful modelling and simulation of a thermoelectric module in TCAD will provide a base for further research into thermoelectric effects, new material structures, module design, and the improvement of thermoelectric efficiency and technology. The aim of the work presented in this chapter is to investigate the basic principle of thermoelectric power generation in the TCAD simulation environment. The initial model, and simulation results presented, successfully demonstrate the fundamental thermoelectric effects, and the concept

of thermoelectric power generation. Future work will build on this initial model, and further analysis of the thermal and electrical simulation results will be published.

This chapter begins with a short background review of thermoelectric technology, followed by an overview of a typical thermoelectric module's construction, highlighting the main elements, material structure, and connection details for thermoelectric power generation.

The chapter then discusses a generic design of a thermoelectric energy harvesting system that incorporates a thermoelectric module with a boost converter, low power DC to DC converter, and a supercapacitor. The 3D modelling of a thermoelectric module is then presented, including the simulation results obtained for the thermal and electrical characteristics of the device when it is connected as a thermoelectric generator. Different thermoelectric couple and module designs have been investigated, and the simulation results have been discussed with reference to fundamental thermoelectric theory. The chapter draws conclusions on the application of thermoelectric technology for energy harvesting, and the validity and effectiveness of the 3D TCAD thermoelectric module simulation model for thermoelectric power generation.

2. Thermoelectric technology

Thermoelectricity utilises the Seebeck, Peltier and Thomson effects that were first observed between 1821 and 1851 [1]. Practical thermoelectric devices emerged in the 1960's and have developed significantly since then with a number of manufacturers now marketing thermoelectric modules for power generation, heating and cooling applications [2]. Ongoing research and advances in thermoelectric materials and manufacturing techniques, enables the technology to make an increasing contribution to address the growing requirement for low power energy sources typically used in energy harvesting and scavenging systems [3]. Commercial thermoelectric modules can be used to generate a small amount of electrical power, typically in the mW or μ W range, if a temperature difference is maintained between two terminals of a thermoelectric module. Alternatively, a thermoelectric module can operate as a heat pump, providing heating or cooling of an object connected to one side of a thermoelectric module if a DC current is applied to the module's input terminals [2].

2.1. Thermoelectric module construction

A single thermoelectric couple is constructed from two 'pellets' of semiconductor material usually made from Bismuth Telluride (Bi_2Te_3). One of these pellets is doped with acceptor impurity to create a P-type pellet, the other is doped with donor impurity to produce an N-type pellet. The two pellets are physically linked together on one side, usually with a small strip of copper, and mounted between two ceramic outer plates that provide electrical isolation and structural integrity. For thermoelectric power generation, if a temperature difference is maintained between two sides of the thermoelectric couple, thermal energy will move through the device with this heat and an electrical voltage, called the Seebeck voltage, will be created. If a resistive load is connected across the thermoelectric couple's output terminals, electrical

current will flow in the load and a voltage will be generated at the load [4]. Practical thermoelectric modules are constructed with several of these thermoelectric couples connected electrically in series and thermally in parallel. Standard thermoelectric modules typically contain a minimum of three couples, rising to one hundred and twenty seven couples for larger devices [2]. A schematic diagram of a single thermoelectric couple connected for thermoelectric power generation, and a side view of a thermoelectric module is shown in Figure 1.

For thermoelectric power generation, a small amount of electrical power can be generated from a thermoelectric module if a temperature difference is maintained between two sides of the module. Normally, one side of the module is attached to a heat source and is referred to as the 'hot' side or 'TH'. The other side of the module is usually attached to a heat sink and is called the 'cold' side or 'TC'. The heat sink is used to create a temperature difference between the hot and cold sides of the module. If a resistive load (RL) is connected across the module's output terminals, electrical power will be generated at the load when a temperature difference exists between the hot and cold sides of the module due to the Seebeck effect [3].

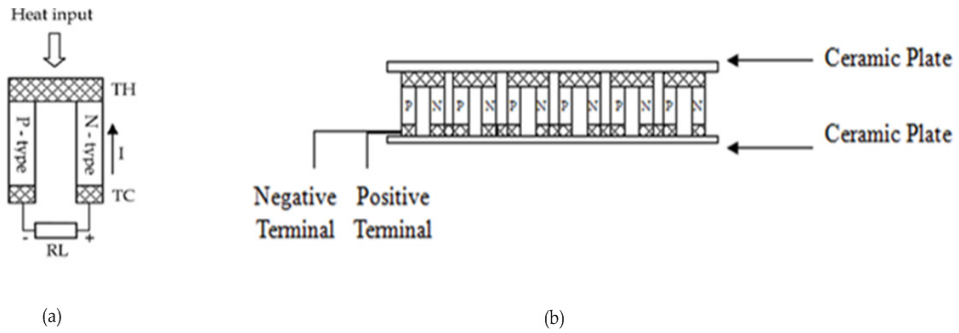


Figure 1. A schematic diagram of a single thermoelectric couple connected for thermoelectric power generation (a), and a side view of a thermoelectric module (b) [5]

A schematic diagram of a thermoelectric module, operating as a thermoelectric power generator, is shown in Figure 2.

The efficiency of a thermoelectric module for power generation can be found by:

$$\eta = \frac{\text{Energy supplied to the load}}{\text{Heat energy absorbed at the hot junction}} \quad (1)$$

In thermoelectricity, efficiency is normally expressed as a function of the temperature over which the device is operated, referred to as the dimensionless thermoelectric figure-of-merit ZT , and can be found by:

$$ZT = \frac{\alpha^2 \sigma}{\lambda} \quad (2)$$

where α is the Seebeck coefficient, σ is the electrical conductivity, and λ is the total thermal conductivity. The best thermoelectric materials used in commercial thermoelectric devices, $\text{Bi}_2\text{Te}_3\text{-Sb}_2\text{Te}_3$ alloys, operating around room temperature, have typical values of $\alpha=225\mu\text{V/K}$, $\sigma = 10^5/\Omega\text{m}$, and $\lambda = 1.5 \text{ W/mK}$, which results in $ZT \approx 1$ [6].

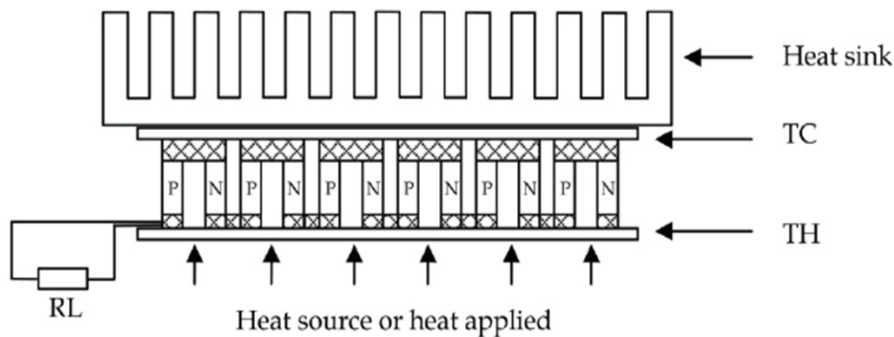


Figure 2. A schematic diagram of a thermoelectric module configured for thermoelectric power generation [5]

3. Thermoelectric energy harvesting

Although the thermoelectric output voltage, current, and electrical power generated by a standard thermoelectric module is relatively small, the thermoelectric output voltage can be boosted to a useful and stable level by using a boost converter and low power DC to DC converter. If the electrical power output from the DC to DC converter is then accumulated and stored for future use in a supercapacitor, it is possible to increase the potential output current of the system, and hence the overall electrical power output of the thermoelectric energy harvesting system. A simplified block diagram of a thermoelectric energy harvesting system is shown in Figure 3. It is not always necessary to use a boost converter, although in many applications, the output voltage from a single thermoelectric module is too low to directly operate a DC to DC converter. The output of the DC to DC converter can also be connected directly to an electrical load in order to power other low power electronic systems, to recharge a battery, or as shown - connected to a supercapacitor for electrical storage purposes. The energy stored in the supercapacitor can then be accumulated over time, and released to the load when required [3]. The addition of the supercapacitor in the system enables much higher levels of current to be drawn by a load, if only for a short period of time, and makes the system more versatile. Commercially available boost converters and low power DC to DC converters can operate from very low thermoelectric output voltages of 20mV, outputting a DC output voltage of between 2.2V to 5V [3].

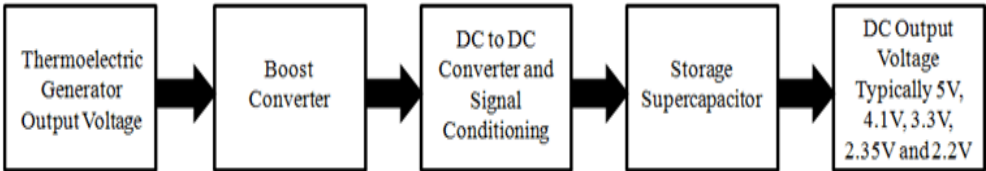


Figure 3. A generic thermoelectric energy harvesting system block diagram [3]

4. Technology Computer Aided Design (TCAD)

The Synopsys TCAD semiconductor simulation package has been chosen for this work as it is widely used in the semiconductor industry to simulate semiconductor device behaviour, and has the capability to simulate the semiconductor manufacturing process in addition to device simulation. Existing published work into thermoelectric modelling and simulation has emphasised the use of ANSYS, COMSOL and Spice compatible software. It is anticipated that modelling a thermoelectric module in TCAD will allow a more detailed analysis of the thermal properties and electrical characteristics of a device than has been published in previous studies. TCAD comprises of a suite of programs that can be executed independently, or together in the form of a Workbench project, in order to simulate the electrical characteristics and thermal properties of a device. Specific TCAD tools have been added to this workbench project in order to create a working simulation. Sentaurus Structure Editor is executed first, and the 3D thermoelectric module is created within this environment, and then meshed using Sentaurus Mesh, followed by device simulation in Sentaurus Device. Tecplot and Inspect have then been used to visualise the results [7].

5. 3D TCAD simulation model of a thermoelectric module containing three thermoelectric couples using Sentaurus Structure Editor

A three couple thermoelectric module has been modelled in Sentaurus Structure Editor, and is shown in Figure 4. The P-type pellets have been simulated using Silicon as the base material, heavily doped with Boron with a constant doping profile and initial concentration of $1 \times 10^{16} \text{ cm}^{-3}$. The N-type pellets are similarly constructed, using Silicon as the base material, heavily doped with Phosphorus at $1 \times 10^{16} \text{ cm}^{-3}$. The seven copper interconnects are labelled 'Copper Connect 1' through to 'Copper Connect 7' respectively. An electrode contact was made on the face of Copper 2 and Copper 7 to simulate the negative and positive electrical connections to the couple, and is shown in Figure 5. A thermal contact was made on the faces of Copper 1 through to Copper 7 respectively, in order to allow the temperature of each contact to be specified or calculated, and the dimension of the 3D device in the Z-direction is 1100 micron metres. Although most commercial thermoelectric modules use Bismuth Telluride as the base material, as this exhibits the most pronounced thermoelectric effects at room temperature, this work has used Silicon as the base material for simulation. TCAD's physical device equations that describe the carrier distribution and conduction mechanisms, materials database and parameter list is comprehensive for Silicon. Once the basic thermoelectric properties have been successfully demonstrated using Silicon, even though this may be at a reduced level than could be seen with state-of-the-art materials, it will be possible to alter the material structure and move to Bismuth Telluride and other material structures with increased confidence.

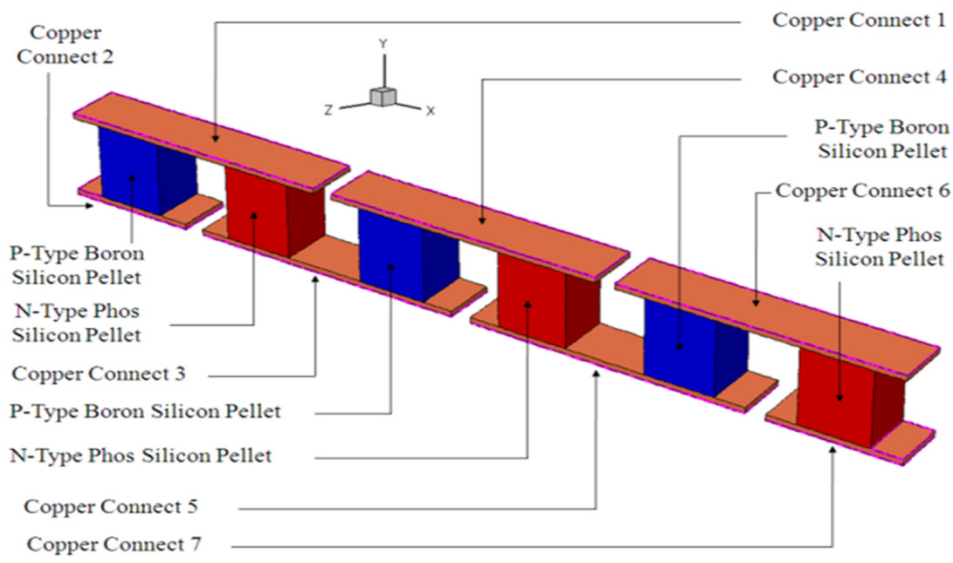


Figure 4. 3D three couple thermoelectric module modelled in Sentaurus Structure Editor [8]

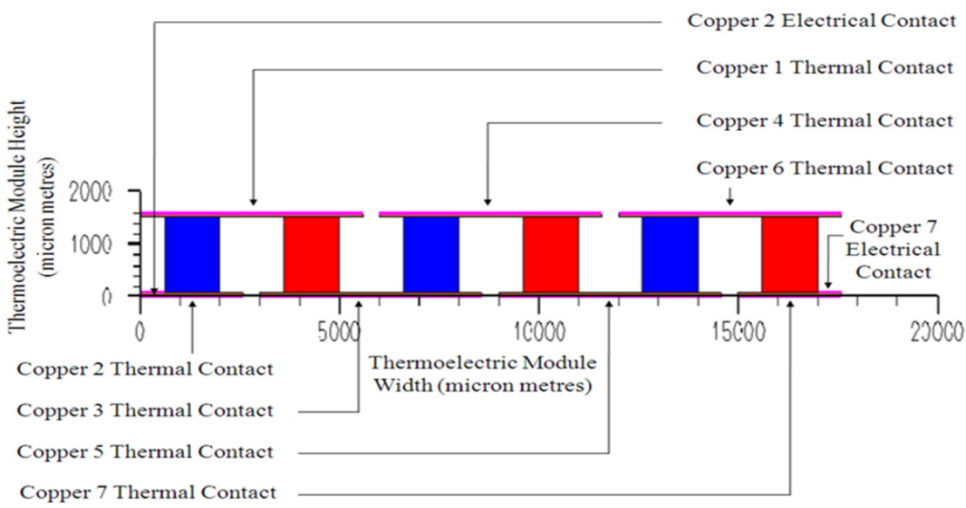


Figure 5. A cut-through in the Z direction highlighting the thermal and electrical connections [8]

The 3D thermoelectric module model was simulated as a TCAD ‘Mixed Mode Simulation’ rather than a ‘Single Device Simulation’, as it is possible to add external components and circuitry to the 3D device structure designed in Sentaurus Structure Editor. In this case a load resistor (R_L) was connected between the electrical output terminals ‘Copper 2’ and ‘Copper 7’ of the device, as shown in Figure 6, in order to calculate the electrical power generated at the load. A three couple thermoelectric module with ceramic outer plates has

also been simulated, and is shown in Figure 7 and Figure 8. The top and bottom face of the two ceramic plates have been used as the thermal contacts of the device, and are labelled 'Ceramic top' and 'Ceramic bottom' respectively. Otherwise, the construction of the device is the same as shown earlier for a three couple thermoelectric module without ceramic outer plates [8].

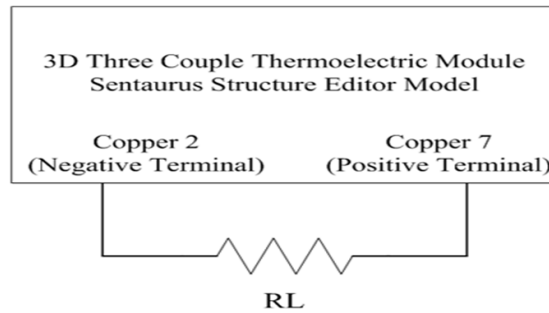


Figure 6. A schematic representation of a TCAD Mixed Mode simulation of a thermoelectric module with a load resistance RL connected between the thermoelectric model output terminals [8]

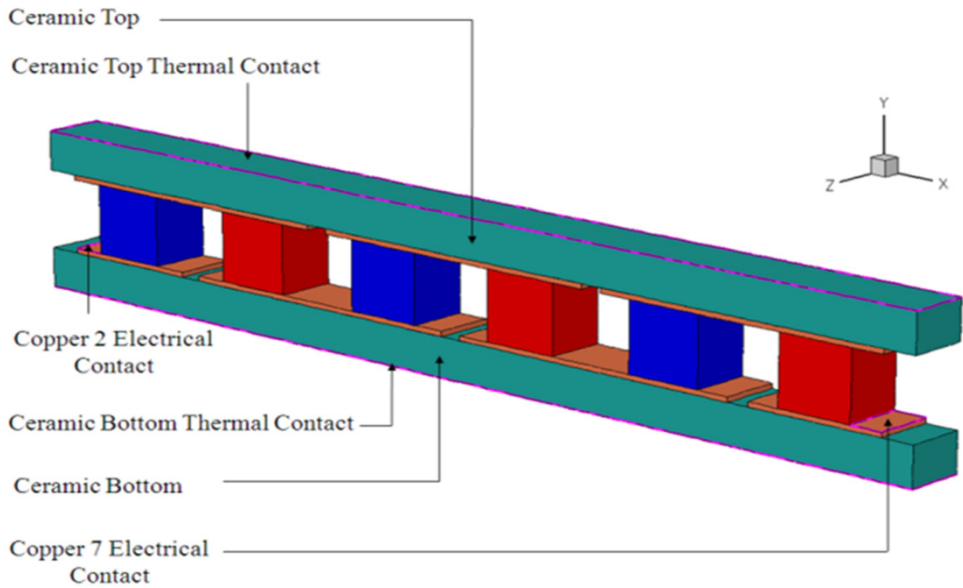


Figure 7. A 3D three couple thermoelectric module with ceramic outer plates modelled in Sentaurus Structure Editor [8]

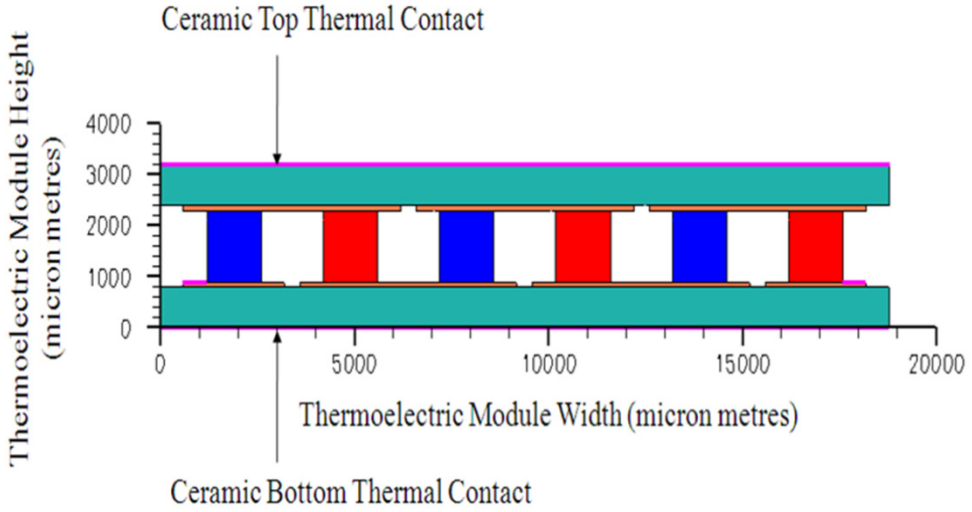


Figure 8. A cut-through in the Z direction highlighting the thermal connections [8]

6. Simulation methodology

The three couple thermoelectric module has been modelled in Sentaurus Structure Editor, connected to a load resistor R_L , and tested using a Mixed Mode simulation for thermoelectric power generation. The temperature of the thermal contacts; Copper 1; Copper 4; and Copper 6; was increased from steady-state conditions of 300 Kelvin to 301 Kelvin. The temperature of the other four thermal contacts; Copper 2; Copper 3; Copper 5; and Copper 7; were kept at 300 Kelvin. This creates a 1 Kelvin temperature difference between both sides of the module. The load resistance R_L was increased from 10 ohms through to 150 ohms, in 10 ohm steps, in order to establish where maximum power is generated at the load. The voltage across the load resistor, and the load current, was recorded using the simulation program, and the electrical power generated at the load calculated using:

$$P = V \times I \text{ measured in Watts} \quad (3)$$

where V is the electrical voltage measured across the load resistor R_L , and I is the electrical current flowing through the load resistor R_L . The P-type and N-type doping concentration was altered from $1 \times 10^{16} \text{cm}^{-3}$ to $1 \times 10^{15} \text{cm}^{-3}$ and $1 \times 10^{17} \text{cm}^{-3}$ in order to establish if the doping concentration has any effect on the electrical power generated by the thermoelectric module. The temperature of the thermal contacts; Copper 1; Copper 4; and Copper 6; was then increased from 301 Kelvin to 325 Kelvin; 350 Kelvin; 375 Kelvin; and 400 Kelvin. The temperature of the other four thermal contacts; Copper 2; Copper 3; Copper 5; and Copper 7; were kept at 300 Kelvin. This creates a temperature difference between both sides of the module of 25 Kelvin; 50 Kelvin; 75 Kelvin; and 100 Kelvin respectively. The simulation was

then repeated using the model of a three couple thermoelectric module with ceramic outer plates for comparison [8].

7. Simulation results

For thermoelectric power generation, the simulation results successfully demonstrate that if the thermoelectric module is subjected to a temperature gradient from one side of the device to the other, electrical power is generated at the load resistor R_L connected between the device output terminals. This is in agreement with the fundamental thermoelectric theory discussed earlier. With an initial doping concentration of $1e+16\text{cm}^{-3}$ for the P-type and N-type silicon pellets, and a temperature gradient of 1 Kelvin across the device, the lattice temperature of the module is shown in Figure 9, and the electrical power generated at the load shown in Figure 10. The maximum power generated at the load occurs with a load resistance of 50 ohms, and a peak power at the load of 0.1 micro-watts. Further tests have been conducted with a modified P-type and N-type doping concentration of $1e+15\text{cm}^{-3}$, $1e+16\text{cm}^{-3}$, and $1e+17\text{cm}^{-3}$, with the results shown in Figure 11. Changing the doping concentration significantly alters the amount of electrical power generated at the load, and the resistance of the device where maximum power is observed. The doping concentration can be optimised to achieve maximum power generation, and a full set of test results will be published. Increasing the thermal gradient on both sides of the device, by increasing the temperature of the thermal contacts at Copper 1, Copper 4 and Copper 6, results in an increase in electrical power generated at the load, as shown in Figure 12. This is as expected as the Seebeck effect is temperature dependent, and the electrical power generated by a thermoelectric module is related to the temperature gradient between two sides of the device [2]. The lattice temperature of the thermoelectric module, with an applied 100 Kelvin temperature gradient between both sides of the device, is shown in Figure 13 and demonstrates that the temperature gradient within each individual thermoelectric P-type and N-type pellet, is now significantly higher than was obtained with a much lower temperature gradient of 1 Kelvin applied to the device in Figure 9 [8].

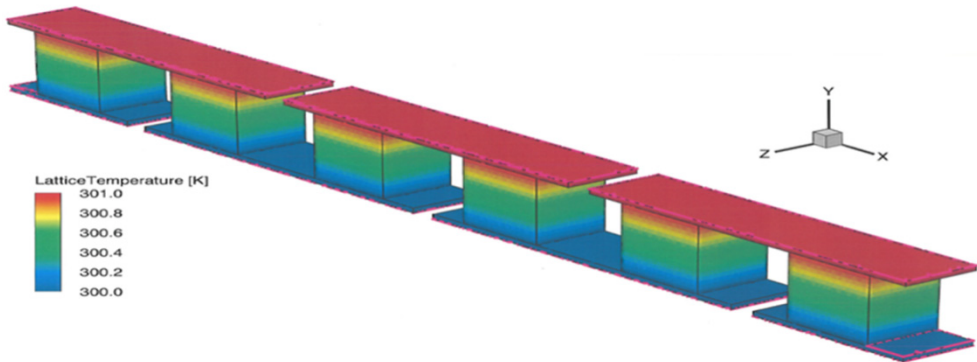


Figure 9. The lattice temperature of the thermoelectric module with an applied 1 Kelvin temperature gradient between both sides of the module [8]

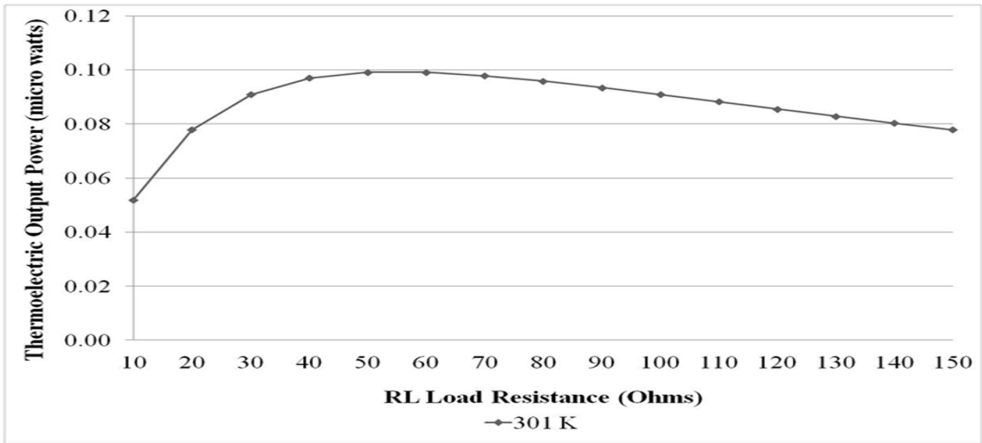


Figure 10. The electrical power generated at the load resistor (RL) with an applied 1 Kelvin temperature gradient between both sides of the module [8]

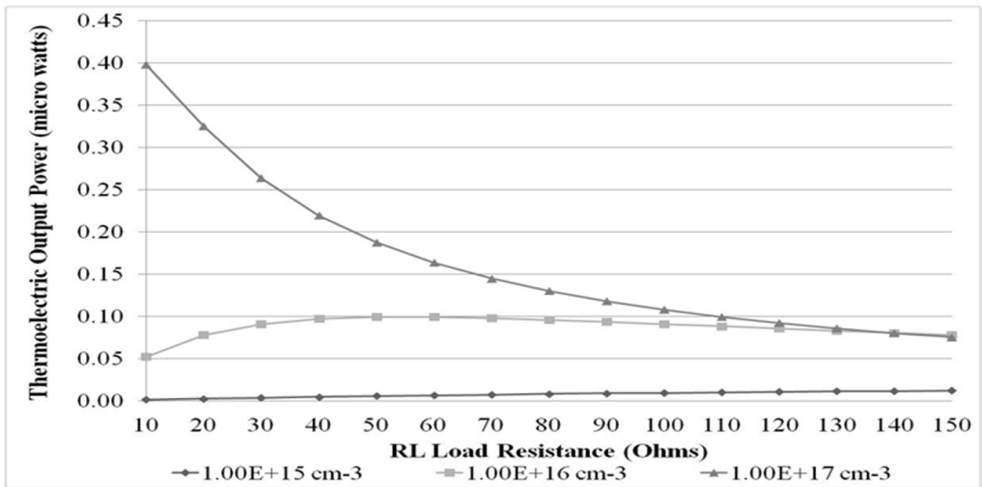


Figure 11. The electrical power generated at the load resistor (RL) with a 1 Kelvin temperature gradient and different P-type and N-type doping concentrations [8]

The simulation has been repeated on the thermoelectric module with ceramic outer plates, shown earlier in Figure 7 and Figure 8. With a 1 Kelvin temperature gradient applied to the module, and a doping concentration of $1\text{e}^{+16}\text{cm}^{-3}$, the ceramic outer plates absorb some of the applied temperature gradient, and the temperature gradient within the thermoelectric pellets is now more uniform than observed earlier, shown in Figure 14. This has the effect of reducing the electrical power generated at the load, shown in Figure 15. However, the ceramic plates are necessary in practical thermoelectric devices in order to create electrical isolation and provide a foundation to mount the thermoelectric couples. The thermal

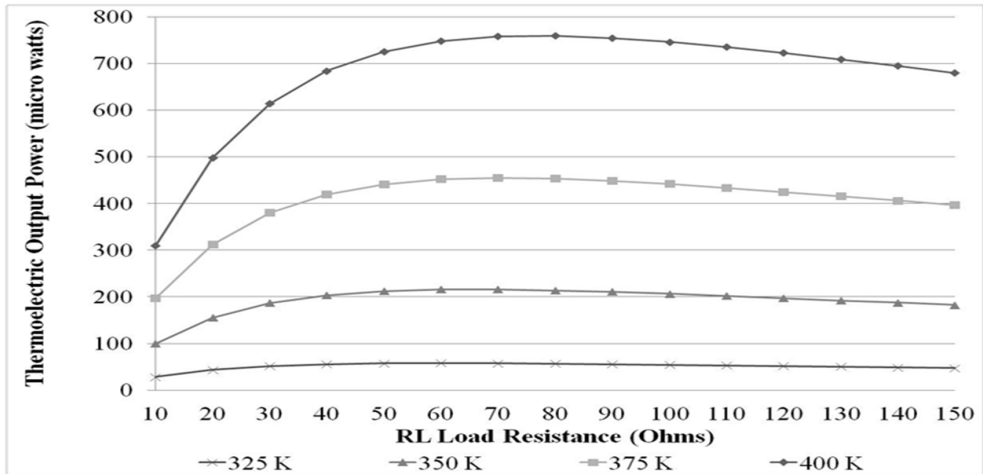


Figure 12. The electrical power generated at the load resistor (RL) with a doping concentration of $1 \times 10^{16} \text{ cm}^{-3}$ and different temperature settings applied to the thermal contacts Copper 1, Copper 4 and Copper 6 [8]

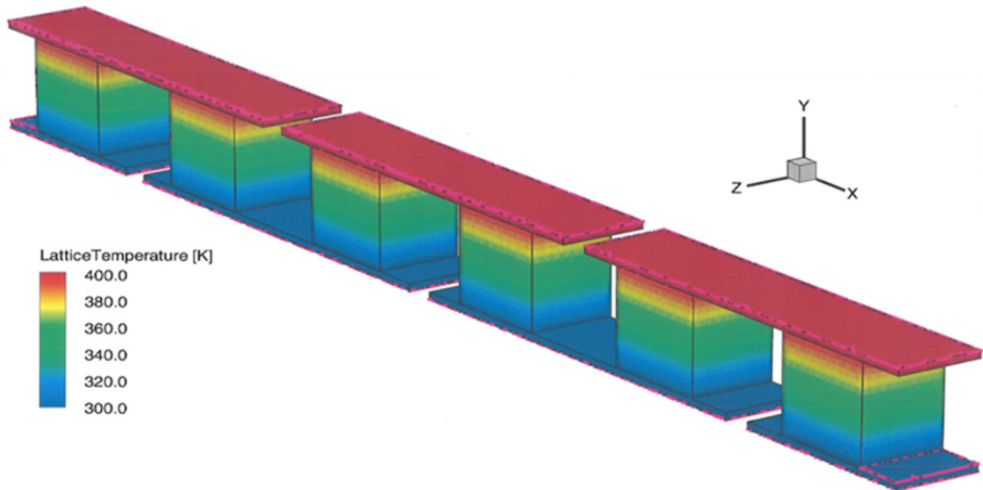


Figure 13. The lattice temperature of the thermoelectric module with an applied 100 Kelvin temperature gradient between both sides of the module [8]

conductivity of the ceramic used in the simulation model is 0.167 [W/ cm K] . Practical thermoelectric modules optimise the thermal conductivity of the ceramic used in the construction of the outer plates, and are typically constructed using Alumina ceramics [9]. Optimising the material properties of the ceramic outer plates used in the simulation model, by increasing their thermal conductivity, should improve the electrical power generated by the thermoelectric module.

The TCAD simulation results demonstrate the basic principle of thermoelectric power generation. The use of Silicon as the base material is sufficient to demonstrate the fundamental concepts, although the output power of the thermoelectric simulation model is much lower than would be expected from a practical thermoelectric module that was manufactured with Bismuth Telluride. This is not unexpected, as Silicon has a far lower Seebeck coefficient than Bismuth Telluride. Future work will investigate different material structures, novel module design and technology, and the results will be published.

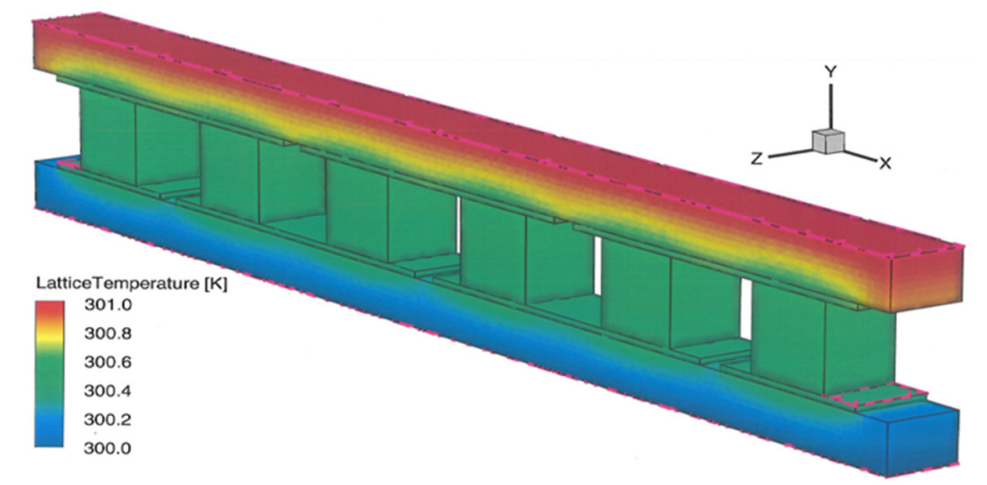


Figure 14. The lattice temperature of the thermoelectric module with ceramic outer plates and an applied 1 Kelvin temperature gradient between both sides of the module [8]

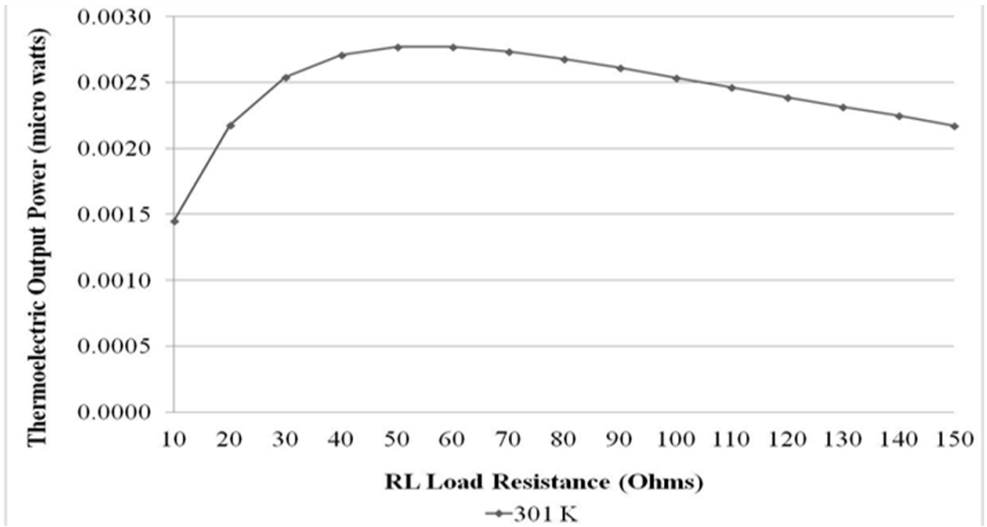


Figure 15. The electrical power generated at the load with an applied 1 Kelvin temperature gradient between both sides of the module [8]

8. Conclusions

Thermoelectric technology is ideally suited as a low power energy source for thermal energy harvesting systems, and with the addition of a boost converter and low power DC to DC conversion, coupled with electrical energy storage in supercapacitors, it is possible to construct a thermoelectric energy harvesting system capable of supplying electrical power to other low power electronic systems, and replace or recharge batteries in several applications. The 3D simulation of a three couple thermoelectric module in TCAD has been successfully achieved, and the simulation results demonstrate the basic principle of thermoelectric power generation. The use of Silicon as the base material is sufficient to demonstrate the basic concepts, and the TCAD thermoelectric simulation model can be used for further analysis into thermoelectric effects, material structure, module design and technology.

Author details

Chris Gould and Noel Shammass

Faculty of Computing, Engineering and Technology, Staffordshire University, Stafford, United Kingdom

9. References

- [1] G. S. Nolas, J. Sharp, H. J. Goldsmid, *Thermoelectrics – Basic Principles and New Materials Developments*, Springer-Verlag, 2001, pp. 1-5
- [2] D. M. Rowe, "General Principles and Basic Considerations", in *Thermoelectric Handbook – Macro to Nano*, D. M. Rowe (Ed.), CRC Taylor & Francis Group, 2006, pp. 1-10
- [3] C. A. Gould, N. Y. A. Shammass, S. Grainger, I. Taylor, "Thermoelectric power generation: Properties, application and novel TCAD simulation", *14th IEEE European Conference on Power Electronics and Applications (EPE2011)*, Aug 30th to 1st Sept 2011, Birmingham, UK, pp. 1-10
- [4] C. M. Bhandari, "Thermoelectric Transport Theory", in *CRC Handbook of Thermoelectrics*, D. M. Rowe (Ed), CRC Taylor & Francis Group, 1995, pp. 27-42
- [5] Chris Gould, Noel Shammass, "A Review of Thermoelectric MEMS Devices for Micro-power Generation, Heating and Cooling Systems", in *Micro Electronic and Mechanical Systems*, Kenichi Takahata (Ed.), INTECH, 2009, pp. 15 – 24, ISBN 978-953-307-027-8
- [6] B. C. Sales, "Critical review of recent approaches to improved thermoelectric materials", *International Journal of Applied Ceramic Technology*, vol. 4, no. 4, August 2007, pp. 291-296
- [7] C. A. Gould, N. Y. A. Shammass, S. Grainger, I. Taylor, "A Novel 2D TCAD Simulation of a Thermoelectric Couple", *Proc. of ECT2010 – 8th European Conference on Thermoelectrics*, Sept 22nd to 24th 2010, Como, Italy, pp. 239-243
- [8] C. A. Gould, N. Y. A. Shammass, S. Grainger, I. Taylor, "A 3D TCAD Thermal and Electrical Simulation of a Thermoelectric Module configured for Thermoelectric Power

- Generation", *9th IEEE International Microtherm Conference*, Lodz, Poland, 28th June – 1st July 2011, pp. 1 – 6
- [9] R. Marlow, E. Burke, "Module Design and Fabrication", in *CRC Handbook of Thermoelectrics*, D. M. Rowe (Ed.), CRC Taylor & Francis Group, 1995, pp. 597 - 607