# A novel 3D TCAD simulation of a thermoelectric couple configured for thermoelectric power generation

C.A. Gould, N.Y.A. Shammas, S. Grainger, I. Taylor

Staffordshire University (UK)

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# Objectives

- Create a 3D model of a single thermoelectric couple using Synopsys Technology Computer Aided Design (TCAD) semiconductor design software

- Simulate the electrical and thermal behaviour of the 3D thermoelectric couple model

- Demonstrate the basic thermoelectric effects and present the simulation results for thermoelectric power generation

# Thermoelectric power generation

The concept of using thermoelectric technology to generate electrical power from naturally occurring heat sources, and waste heat in a system, has been considered for some time, although the technology is often overlooked in discussions surrounding renewable energy sources

Partly due to the relatively low levels of electrical power generated from a single thermoelectric module, and a typical conversion efficiency of between 5% to 10%

Higher levels of electrical power can be output from a thermoelectric power generation system if several modules are connected together in series or parallel

The technology is considered an environmentally friendly and renewable energy source, and can be used in applications where other renewable technologies could not be used, or in combination with other renewable technologies, in order to enhance a system’s overall performance

# Thermoelectric power generation

Recent focus and research has increased significantly in the area of low-power energy harvesting systems

Parallel developments in:

Low-power DC to DC conversion techniques
Electrical energy storage in supercapacitors

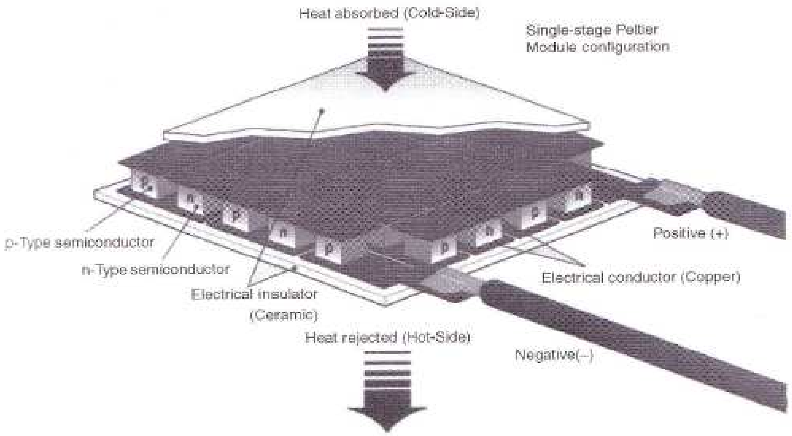
Thermoelectricity can make a major contribution to the development of low-power energy sources, and by using low-power DC to DC conversion and supercapacitors, can output sufficient electrical power to operate low-power electronic systems, and recharge or replace batteries in many applications

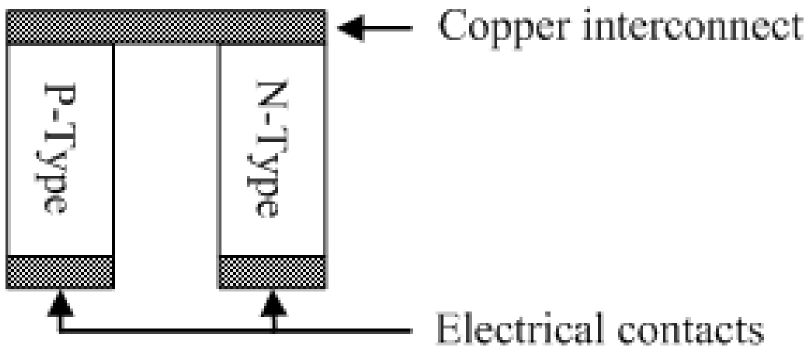
The technology is not limited to low-power applications:

Power source for space-craft for deep-space missions

Developing market in the automotive sector for thermoelectric power generation from vehicle waste heat (around 200W to 300W)

# Fundamental thermoelectric theory



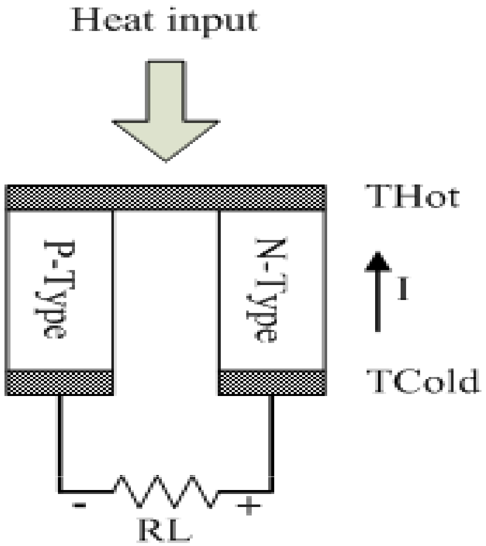



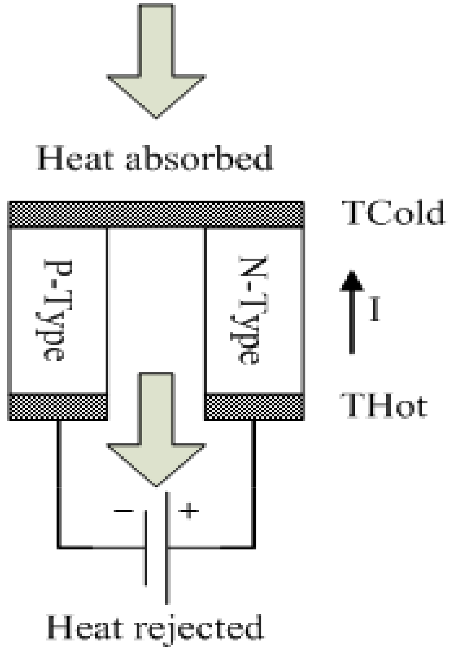

A standard thermoelectric module is typically constructed from several P-type and N-type thermoelectric couples

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 placed between two ceramic plates

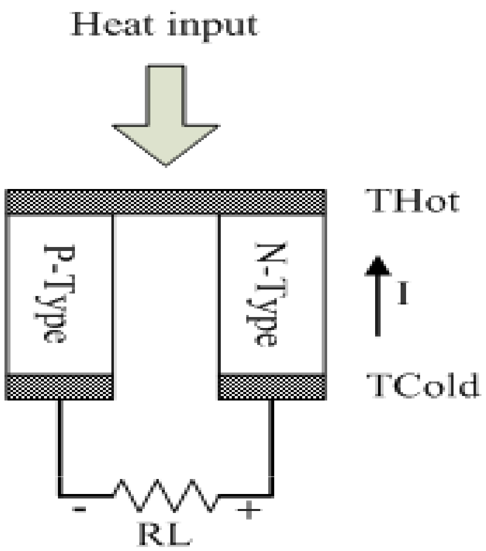



A small amount of electrical power, typically in the μW range, can be generated by a single thermoelectric couple if a temperature difference is maintained between two sides of the couple

A single thermoelectric couple can operate as a heat-pump, providing cooling or heating of an object connected to one side of the couple if a DC current is applied to the couple's input terminals

# Thermoelectric power generation

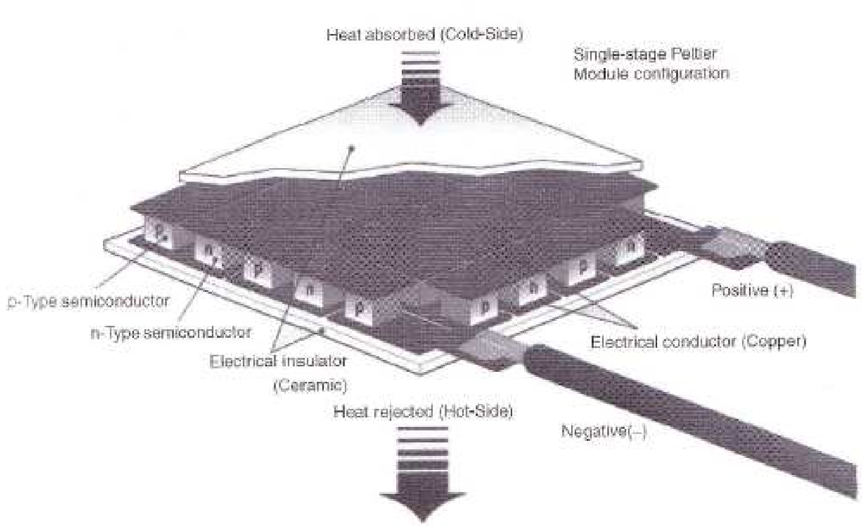



If a temperature difference is maintained between two sides of the thermoelectric couple, thermal energy will move through the electrically conductive N-type and P-type pellets

Charge carriers 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 module's output terminals, electrical current will flow in the load and a voltage will be generated at the load

# Typical thermoelectric module




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 a larger device

# Technology Computer Aided Design (TCAD)

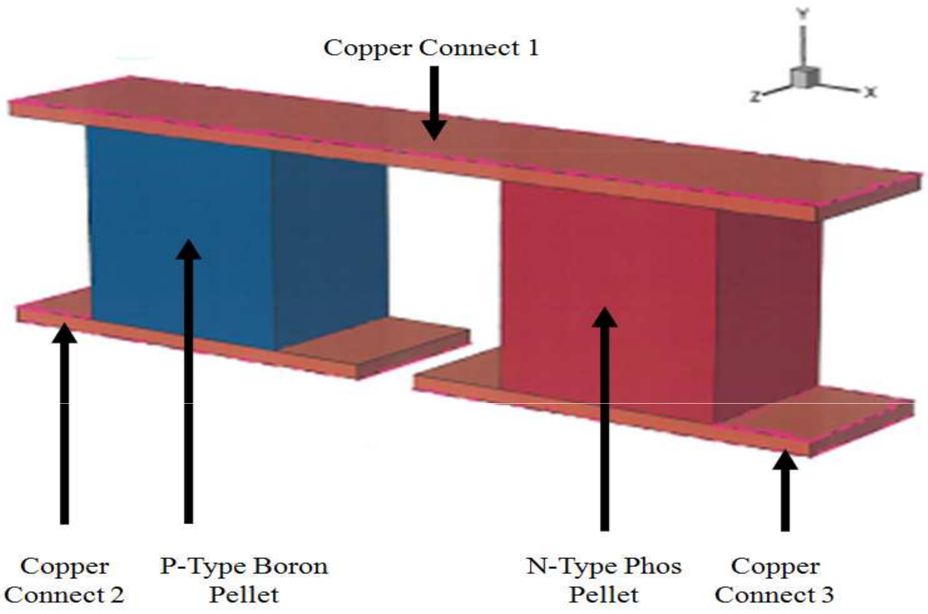
The Synopsys TCAD semiconductor simulation package has been chosen for this work as it is widely used in the semiconductor industry to simulate semiconductor device behaviour, and has the capability to simulate the semiconductor manufacturing process in addition to device simulation

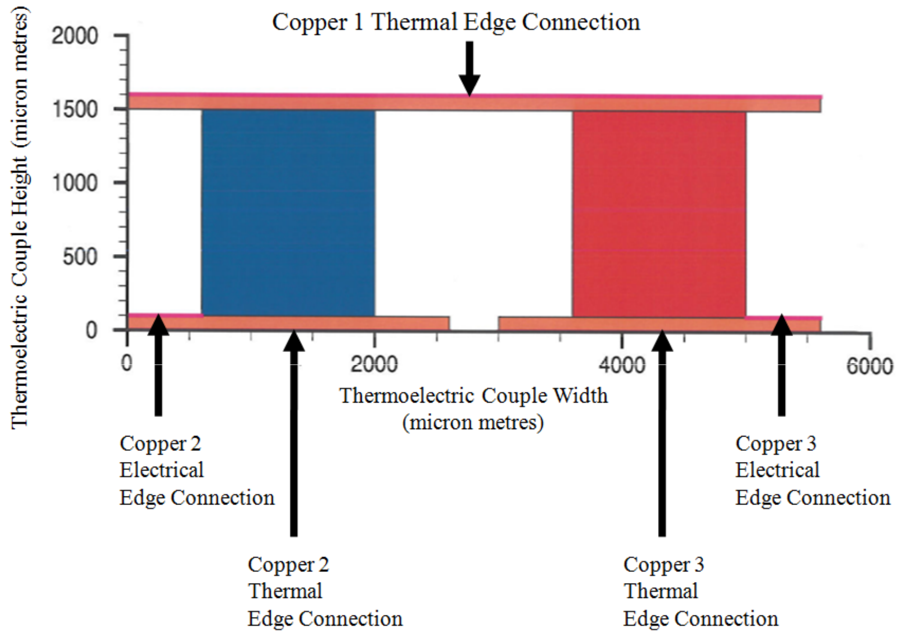
Existing published work into thermoelectric modelling and simulation have emphasised the use of ANSYS, COMSOL and SPICE compatible simulation software

This is the first time TCAD has been used to model and simulate a P-N Couple rather than a P-N Junction

The successful modelling of a single thermoelectric couple in TCAD will allow a more detailed analysis of the thermoelectric electrical and thermal effects to be undertaken than has been published in previous studies

# 3D TCAD thermoelectric couple model

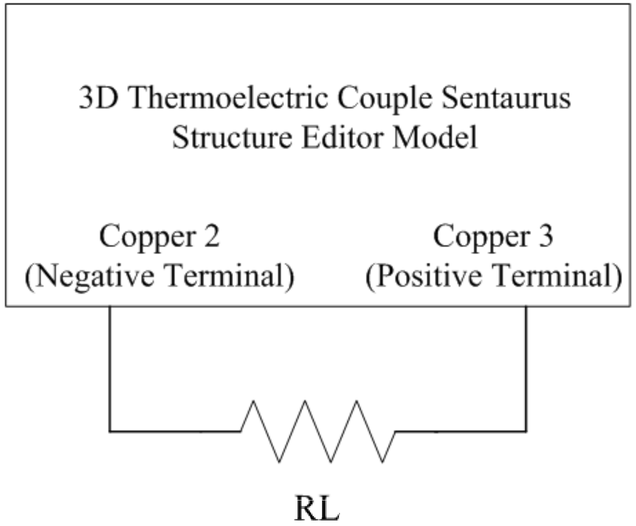



A single thermoelectric couple has been modelled in TCAD

The P-type and N-type material has been simulated using Silicon as the base material

# Mixed mode simulation

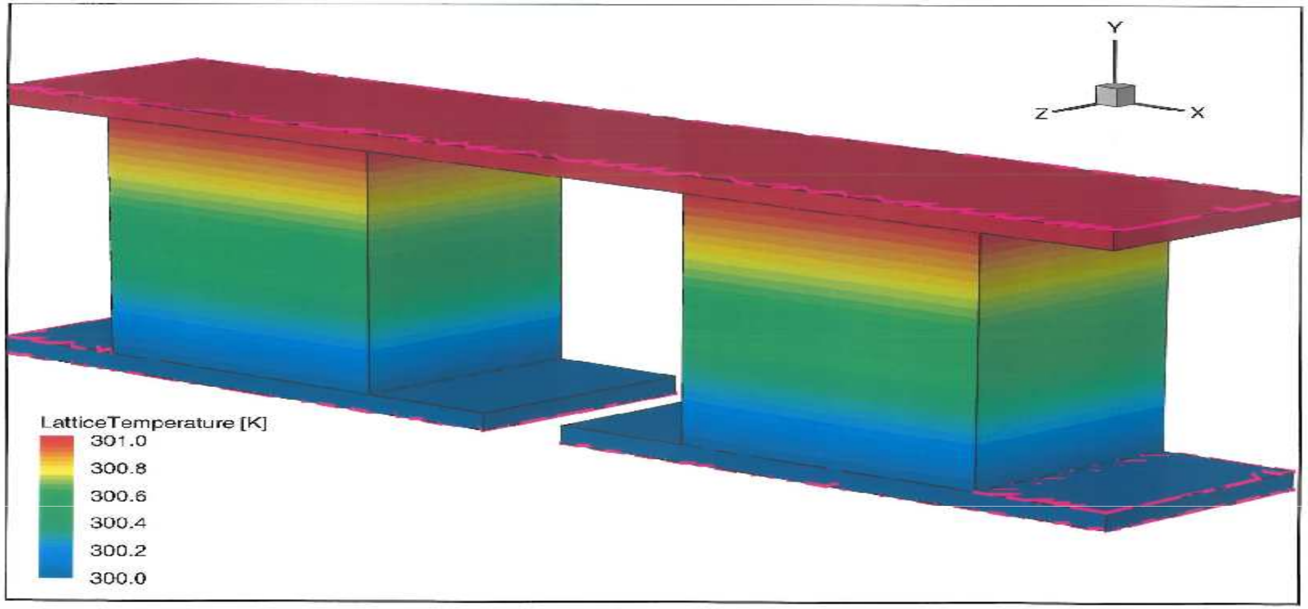



For thermoelectric power generation, the 3D thermoelectric couple was simulated as a TCAD 'Mixed Mode Simulation' rather than a 'Single Device Simulation'

In Mixed Mode simulation, it is possible to add external components and circuitry

A load resistor (RL) was connected between the output terminals 'Copper 2' and 'Copper 3' of the device, in order to calculate the electrical power generated at the load

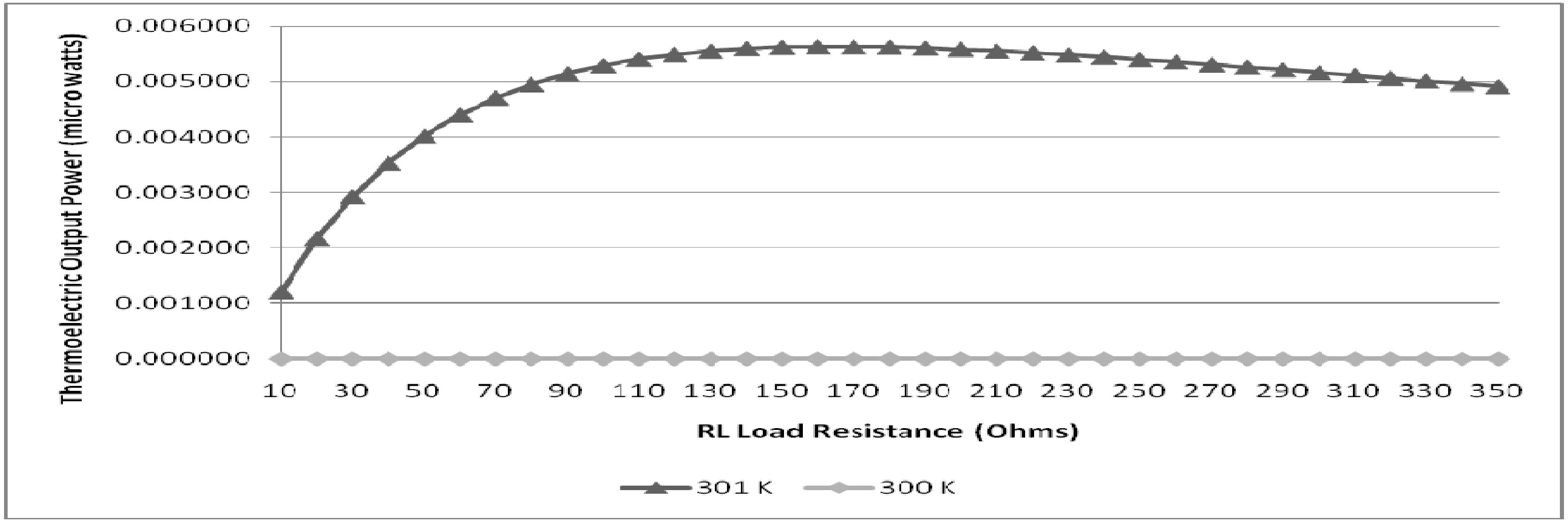
# Results




With an initial doping concentration of $1e^{+}15cm^{-3}$ for both P-type and N-type pellets, the temperature of the thermal connection at Copper 1 was increased from 300 Kelvin to 301 Kelvin, with the temperature of the thermal contacts at Copper 2 and Copper 3 maintained at 300 Kelvin

The temperature of the thermoelectric couple's lattice is shown under these test conditions, and highlights that a temperature gradient exists within the device

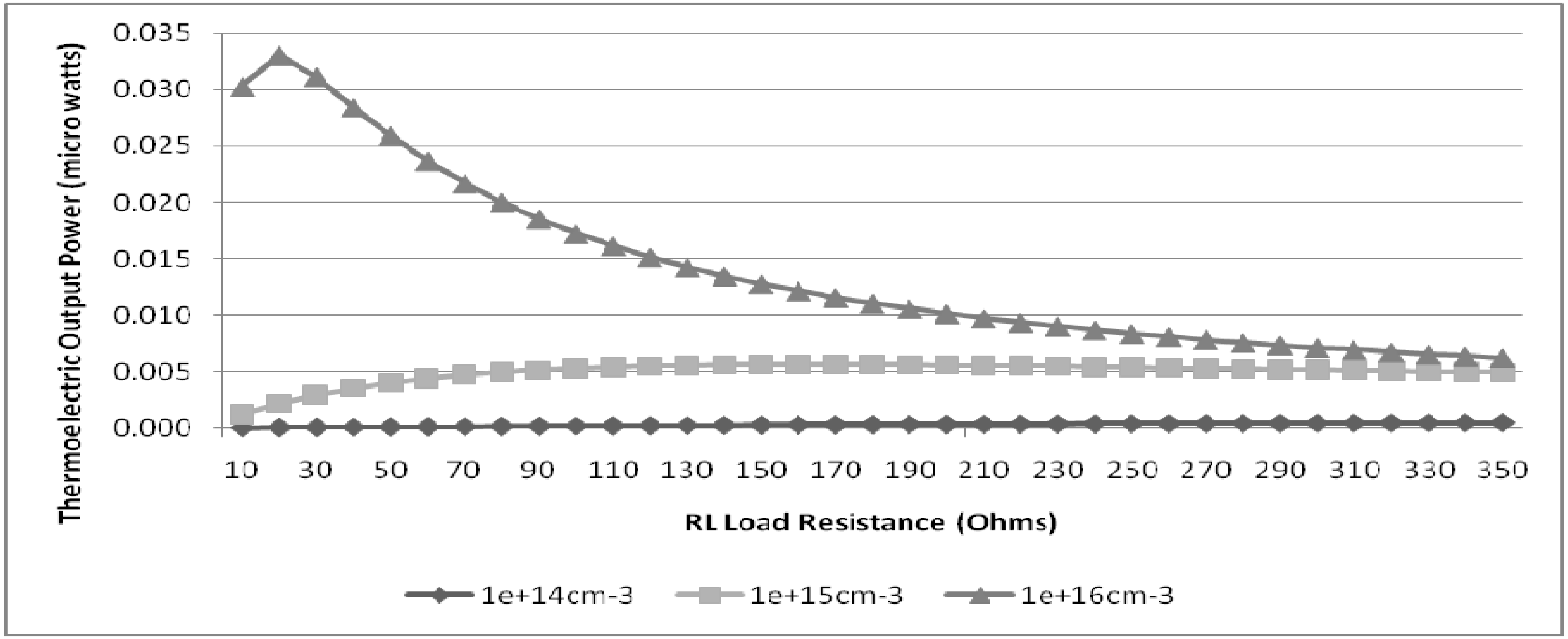
# Results




It can be seen that without a temperature gradient, there is only negligible electrical power generated at the load, although it is not absolutely zero watts

As the temperature gradient of 1 Kelvin is applied to the device, the output power at the load can be seen to increase to a peak of 0.00563 micro watts with a load resistance of 170 ohms, where maximum power transfer is achieved

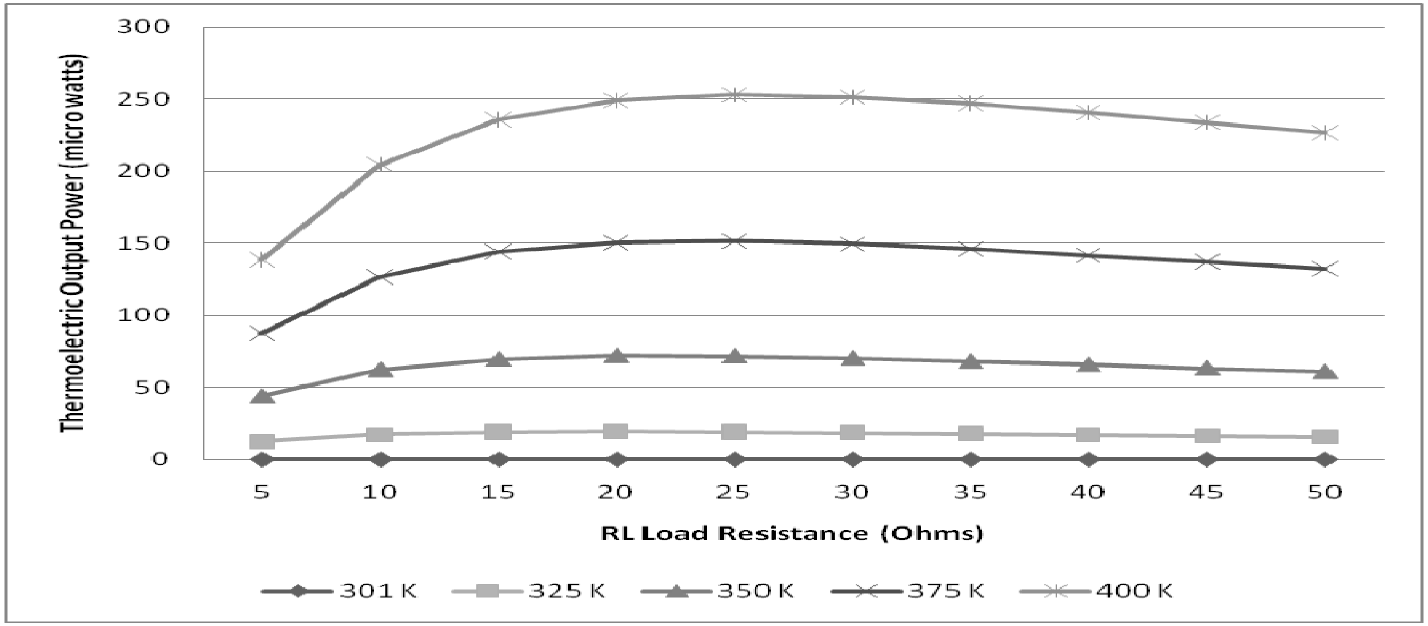
# Results




Changing the doping concentration significantly alters the amount of electrical power generated at the load, and the internal resistance of the device

As the internal resistance of the device has now changed, the value of load resistance where maximum power transfer occurs will also change

# Results

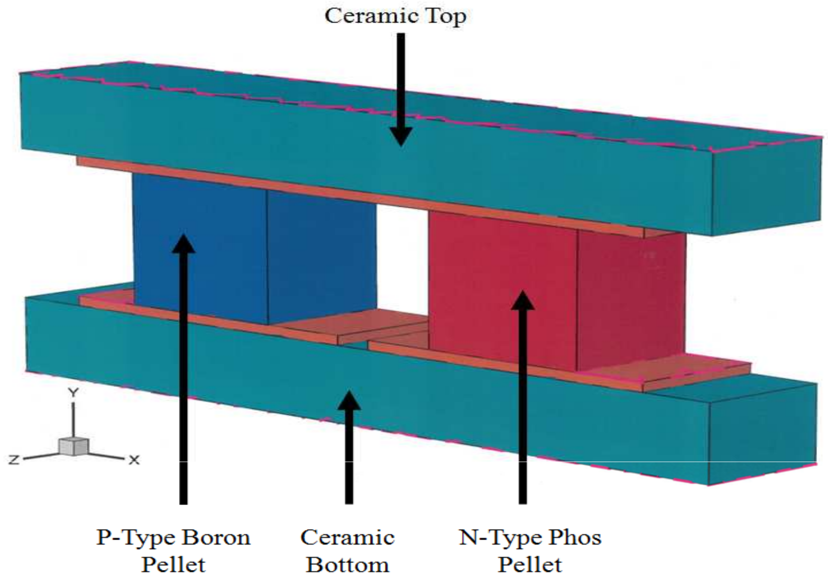


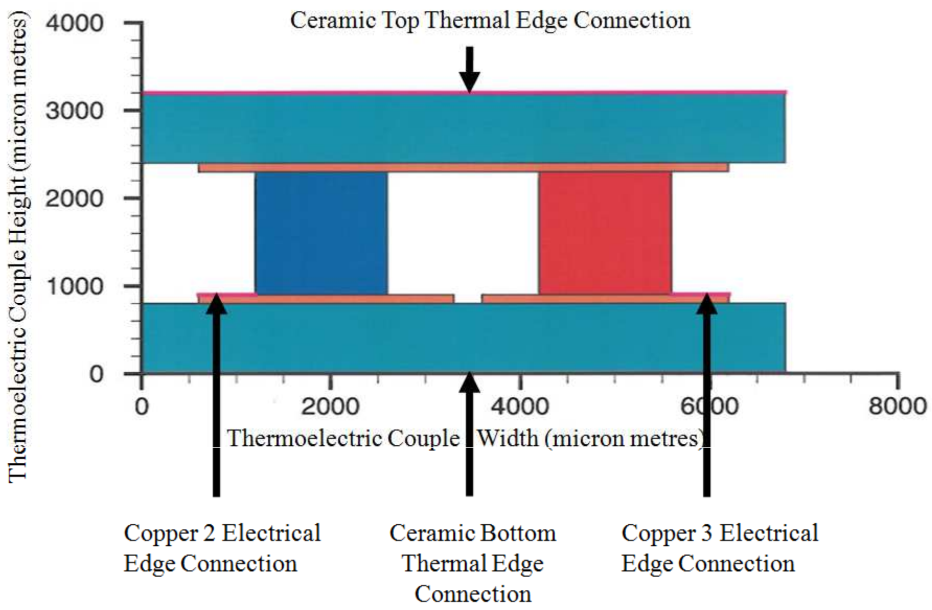

Increasing the thermal gradient on both sides of the device, by increasing the temperature of the thermal contact at Copper 1, results in an increase in electrical power generated at the load

This is as expected as the Seebeck effect is temperature dependent

A doping concentration of $1e^{+}16cm^{-3}$ for both P-type and N-type pellets was used for these tests

# 3D TCAD thermoelectric couple model with ceramic outer plates

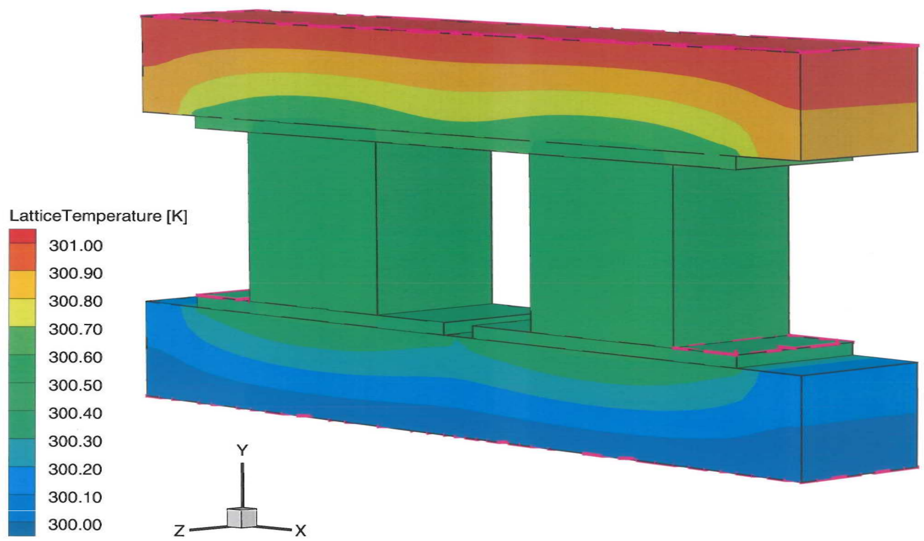



The top and bottom face of the two ceramic plates have been used as the thermal contacts of the device, and are labelled 'Ceramic top' and 'Ceramic bottom' respectively

Otherwise, the construction of the device is the same as shown earlier for a single thermoelectric couple

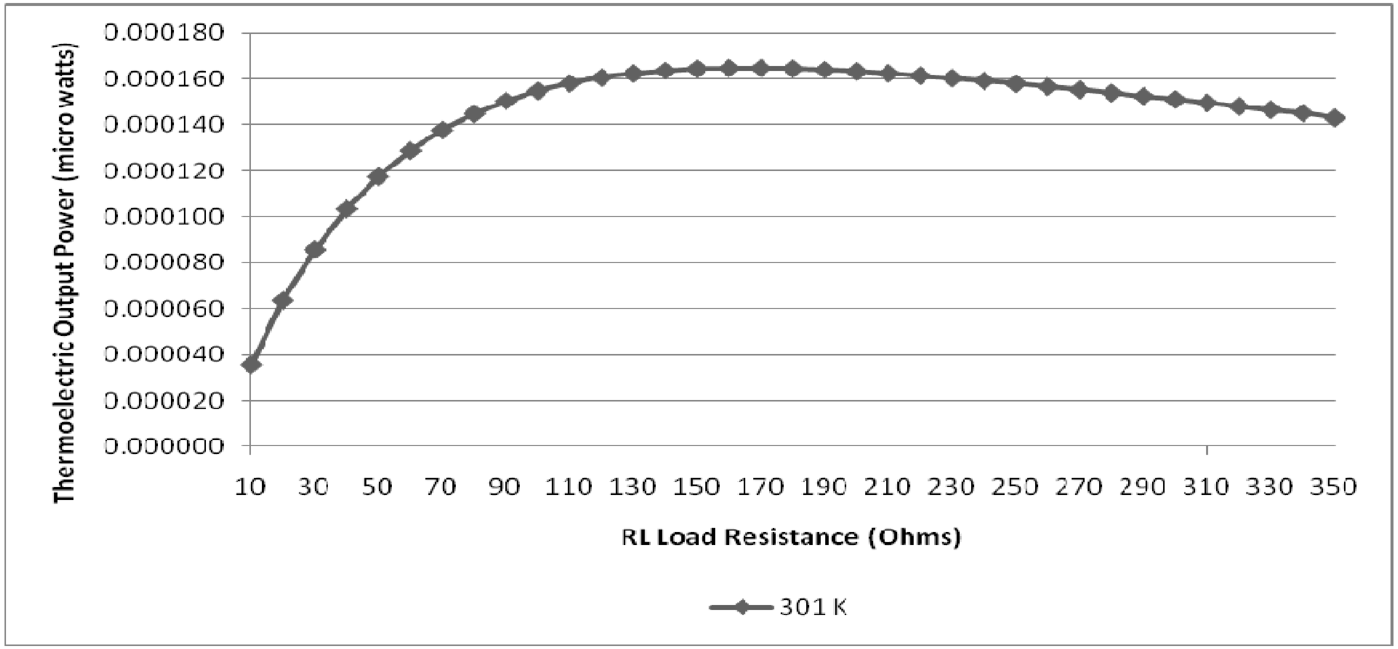
# Results




The temperature of the thermal connection at ‘Ceramic Top’ was increased from 300 Kelvin to 301 Kelvin, with the temperature of the thermal contact at ‘Ceramic Bottom’ maintained at 300 Kelvin

The ceramic plates absorb some of the applied temperature gradient, and the temperature gradient within the thermoelectric pellets is now more uniform than shown earlier without the ceramic outer plates

# Results




As the thermoelectric couple is now at a more uniform temperature, the electrical power generated at the load has been reduced when compared to the previous test without the two ceramic plates

Optimising the material properties of the Ceramic used in the construction of the outer plates, by increasing their thermal conductivity, should improve the electrical power generated by the thermoelectric couple

# Conclusions

The 3D simulation of a thermoelectric couple in TCAD has been successfully achieved

The preliminary simulation results demonstrate the basic principle of thermoelectric power generation

The simulation results are in agreement with basic thermoelectric theory, and the use of Silicon as the base material is sufficient to demonstrate the basic concepts

The TCAD thermoelectric couple simulation model can be used for further analysis into thermoelectric effects, material structure and technology

The 3D simulation results presented in this paper confirm the 2D TCAD simulation results obtained in previous simulation experiments and published at ECT2010

C. A. Gould, N. Y. A. Shammas, S. Grainger, I. Taylor, “A Novel 2D TCAD Simulation of a Thermoelectric Couple”, *Proc. of ECT2010 - 8th European Conference on Thermoelectrics*, Sept 22nd-24th 2010, Como, Italy, pp. 239-243