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THE MODELLING AND SIMULATION OF Bi_2Te_3 THERMOELECTRIC GENERATORS IN SYNOPSYS TCAD

This paper demonstrates the modelling and simulation of thermoelectric generators using Synopsys Technology Computer Aided Design (TCAD) semiconductor design and simulation software. A single Bi_2Te_3 thermoelectric couple, and a seven couple Bi_2Te_3 thermoelectric module, have been modelled in Synopsys TCAD and simulated for thermoelectric power generation. The simulation results correctly demonstrate that when a thermoelectric couple or module is subjected to a temperature gradient, electrical power is generated at the load, with higher power levels output as the temperature gradient increases, or as the number of thermoelectric couples contained within the device increases. The simulation results obtained in TCAD, which uses in-built semiconductor physics equations, have been compared to results obtained through numerical calculation using a different set of thermoelectric equations, and the two results are in close agreement. The Synopsys TCAD models can be developed further to investigate novel device structures, and will enable new thermoelectric materials to be investigated within the framework of the simulation environment in an attempt to improve the performance, efficiency, and cost of thermoelectric devices.
Key words: TCAD, modelling and simulation, thermoelectric power generation.

Introduction

The use of computer based modelling and simulation techniques in the design of commercial thermoelectric modules is limited, with numerical calculation and bulk semiconductor manufacturing techniques common practice. This is partly due to the large geometry size of the modules, and the use of bulk semiconductor material such as Bismuth Telluride in the construction of the thermoelectric pellets. However, as the industry develops the next generation of micro-thermoelectric devices based on thin-film and nanotechnology, the use of semiconductor design and simulation tools is likely to increase. Published research in the area of thermoelectric modelling and simulation has demonstrated the use of SPICE, ANSYS, and COMSOL, but little evidence can be found for the use of Synopsys TCAD for the modelling and simulation of thermoelectric devices. TCAD is extensively used to model and simulate semiconductor devices in the electronic semiconductor industry, and has the ability to model and simulate the semiconductor manufacturing process, i.e. lithography, deposition, and diffusion, along with 2D and 3D semiconductor device design and electrical and thermal device behaviour. TCAD is very well positioned to be developed as a tool for thermoelectric device modelling and simulation as the next generation of devices, materials, and manufacturing processes converge closer to those seen in the wider electronic semiconductor industry. This paper begins with a brief introduction to Synopsys TCAD, followed by the TCAD modelling and simulation of an *n*-type and *p*-type Bi_2Te_3 pellet, and a single Bi_2Te_3 thermoelectric couple. Simulation results are then presented for the electrical power generated by the thermoelectric couple under different temperature gradients, along with a comparison between the results obtained in the TCAD simulation, and the results obtained by applying a different set of thermoelectric equations. The paper then moves to the

development of a single *Bi$_2$Te$_3$* thermoelectric couple with ceramic outer plates, and a seven couple *Bi$_2$Te$_3$* thermoelectric module. An overall discussion of the work is then presented and appropriate conclusions made.

Computer based modelling and simulation techniques used in the field of thermoelectricity

The aim of this work is to demonstrate that Synopsys TCAD can be used to model and simulate the behaviour of thermoelectric devices when they are configured to operate as a thermoelectric generator. Published work in this area has focused on the use of other simulation packages, notably SPICE, ANSYS, and COMSOL, and this work will identify the advantages, and demonstrate that, Synopsys TCAD can also be used to model and simulate thermoelectric devices. The use of SPICE software has generally focused on the development of a SPICE equivalent circuit model to describe the behaviour of a single thermoelectric couple, or a more generic thermoelectric module or system [1 – 6]. It can be argued that although SPICE equivalent circuit models can be used to describe the behaviour of a thermoelectric couple, module, or system, it is difficult to use this technique as a design aid to develop the next generation of thermoelectric modules that use new materials or device structures, where information on the electrical and thermal performance of the device or system is limited or not readily available. Similarly, ANSYS has been used to take advantage of the relative power of finite-element analysis techniques, with examples amongst others from [7 – 11] describing published work into the modelling and simulation of the power generation and cooling properties of a thermoelectric couple and module in ANSYS. Work in this area has demonstrated that ANSYS is a capable tool for modelling thermoelectric behaviour, with the ability to model device structures in three dimensions, although it is necessary to have a good understanding of the thermoelectric, electrical, and thermal properties of the materials within the device simulation at each temperature of interest before any simulation can be fully executed. The third simulation tool that has recently started to be used by the thermoelectric community is COMSOL, with published work by [12 – 13] demonstrating the modelling and simulation technique for thermoelectric power generation and cooling. The simulation package is similar to ANSYS, in that it uses finite-element analysis, but also allows for direct equation entry when building a simulation model. It is anticipated that successfully modelling a thermoelectric couple and module in Synopsys TCAD will allow for a more detailed electrical and thermal analysis to be made than can currently be achieved by using SPICE, ANSYS or COMSOL.

Synopsys TCAD modelling and simulation

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 semiconductor device. It is a finite-element and SPICE compatible computer simulation program, and solves the fundamental, physical partial differential equations, such as diffusion and transport equations, and supports a broad range of semiconductor applications. A simulation project is first created in Sentaurus Workbench in order to control the flow of the simulation, define experiment parameters and variables. Specific TCAD tools are then added to the Workbench project in order to create a working simulation. Sentaurus Structure Editor is executed first, and a two or three dimensional structure is created within this environment, and then meshed using Sentaurus Mesh. The meshed device is then passed to Sentaurus Device, where the electrical and thermal simulation of the device is executed. The behaviour of the device is simulated numerically by calculating terminal currents, voltage and charges, using a set of physical device equations that describe the carrier distribution and conduction mechanisms, with specific physics models executed according to the models specified within the Sentaurus Device command structure. Sentaurus

device will calculate, amongst others, the; electrostatic potential by solving the semiconductor Poisson equation; continuity equations relating to the thermodynamic carrier transport model; the lattice, electron, and hole temperatures; the electron and hole absolute thermoelectric powers; and the Peltier effect at metal-semiconductor interfaces. The output of Sentaurus Device can then be represented graphically using Sentaurus Visual and Inspect [14]. According to Sentaurus [15], TCAD calculates the electrostatic potential as:

$$\nabla \cdot (\varepsilon \nabla \phi + \vec{p}) = -q(p - n + N_D - N_A) - \rho_{trap},$$ (1)

where ε is the electrical permittivity; $\vec{p}$ is the ferroelectric polarization; q is the elementary electronic charge; n and p are the electron and hole densities; N_D is the concentration of ionized donors; N_A is the concentration of ionized acceptors; and ρ_{trap} is the charge density contributed by traps and fixed charges [15]. The thermodynamic model for current densities accounts for self-heating and includes the temperature gradient as the driving term as:

$$\vec{J}_n = -nq\mu_n(\nabla\Phi_n + P_n\nabla T)$$ (2)

$$\vec{J}_p = -nq\mu_p(\nabla\Phi_p + P_p\nabla T).$$ (3)

where P_n and P_p are the absolute thermoelectric powers, n is the electron density, p is the hole density, q is the elementary electronic charge, μ_n and μ_p are the electron and hole mobility, Φ_n and Φ_p are the electron quasi-Fermi potential and hole quasi-Fermi potential, and T is the lattice temperature [16]. Sentaurus Device can compute up to three different temperatures; lattice temperature; electron temperature; and hole temperature. The lattice temperature describes the self-heating of devices, and within the TCAD environment, the lattice temperature can be computed non-uniformly using the thermodynamic model [17]. According to Sentaurus [18], the electron and hole absolute thermoelectric powers P_n and P_p for nondegenerate semiconductors can be written as:

$$P_n = -k_n\frac{k}{q}\left[\left(\frac{5}{2} - S_n\right) + \ln\left(\frac{N_C}{n}\right)\right],$$ (4)

$$P_p = -k_p\frac{k}{q}\left[\left(\frac{5}{2} - S_p\right) + \ln\left(\frac{N_V}{p}\right)\right],$$ (5)

where the parameters κ_n, κ_p, S_n and S_p can be adjusted in the parameter file. Although the Seebeck effect has the most influence for thermoelectric power generation, it can also be noted that the Peltier effect at metal-semiconductor interfaces is accounted for in TCAD using:

$$Q_n = J_n(\alpha_n\Delta E_n + (1 - \alpha_n)\Delta\varepsilon_n,$$ (6)

$$Q_p = J_p(\alpha_p\Delta E_p + (1 - \alpha_p)\Delta\varepsilon_p,$$ (7)

where Q is the heat density at the interface (when $Q > 0$ there is heating; when $Q < 0$ there is cooling), and J_n and J_p are the electron and hole densities normal to the interface, ΔE_n and ΔE_p are the energy differences for electrons and holes across the interface, and α_n, α_p, $\Delta\varepsilon_n$, and $\Delta\varepsilon_p$ are fitting parameters with $0 \leq \alpha_n$, $\alpha_p \leq 1$ [19].

Background thermoelectric theory

If a single thermoelectric couple, as shown in Fig. 1(*a*), is subjected to a temperature difference between the two two sides of the thermoelectric couple, thermal energy will move through the *p*-type and *n*-type pellets, and as these pellets are electrically conductive, charge carries are transported by this heat. This movement of heat and charge carriers creates an electrical voltage called the Seebeck voltage. If a resistive load is connected across the thermoelectric couple's output terminals, shown in Fig. 1(*b*), current will flow in the load and an electrical voltage will be generated at the load [20]. A single thermoelectric

couple is generally of limited practical use, as the rate of useful power generated due to the Seebeck effect is very small. Practical thermoelectric modules are constructed with several of these thermoelectric couples connected electrically in series and thermally in parallel, with modules typically containing a minimum of three thermoelectric couples, rising to one hundred and twenty seven couples for larger devices [21].
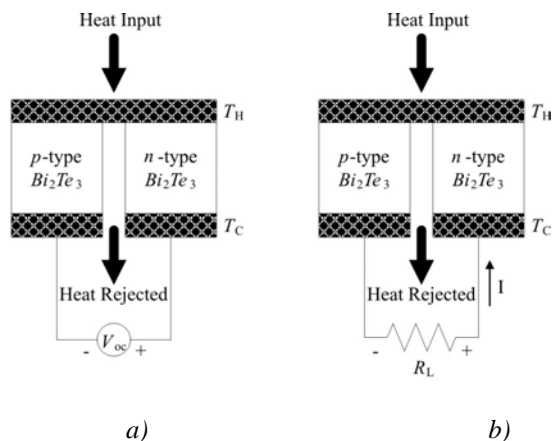

Fig. 1. A single thermoelectric couple configured as a thermoelectric generator with a volt meter measuring the open-circuit voltage V_{oc} (a) and in (b) with a load resistor R_L connected across the couple's output terminals [22].

Synopsys TCAD modelling and simulation of *p*-type and *n*-type *Bi₂Te₃* thermoelectric pellets

Single pellets of both *p*-type and *n*-type Bismuth Telluride (*Bi₂Te₃*) have been modelled in Sentaurus Structure Editor with the material properties given in Table 1, and are typical values used in commercial thermoelectric modules kindly provided by [23]. A single *p*-type *Bi₂Te₃* pellet, shown in Fig. 2 and Fig. 3, has been modelled between two copper connectors, *Copper* 1 and *Copper* 2. These copper connectors act as electrodes for the negative and positive terminals of a DC input voltage source V_{in}. The pellet was simulated at an average temperature of 300.5 K, and as a TCAD mixed-mode simulation. A TCAD compact model voltage source V_{in} of 1 mV was connected between the negative terminal *Copper* 1 and the positive terminal *Copper* 2 of the device, and the resulting circuit current *I* has been measured in TCAD. The pellets electrical resistivity ρ_p, Seebeck coefficient α_p, and thermal conductivity λ_p has also been measured in TCAD, and the pellets resistance R_P calculated. A simulated input voltage V_{in} of 1 mV has then been applied to the input terminals of each pellet resulting in a circuit current *I* of 104.51 mA. The pellets properties with an average pellet temperature of; 300.5 K; 312.5 K; 325 K; 337.5 K; and 350 K; are summarised in Table 2.
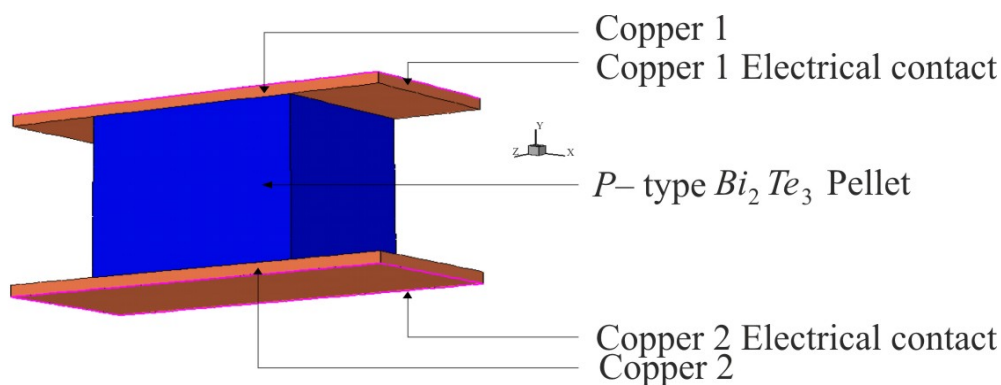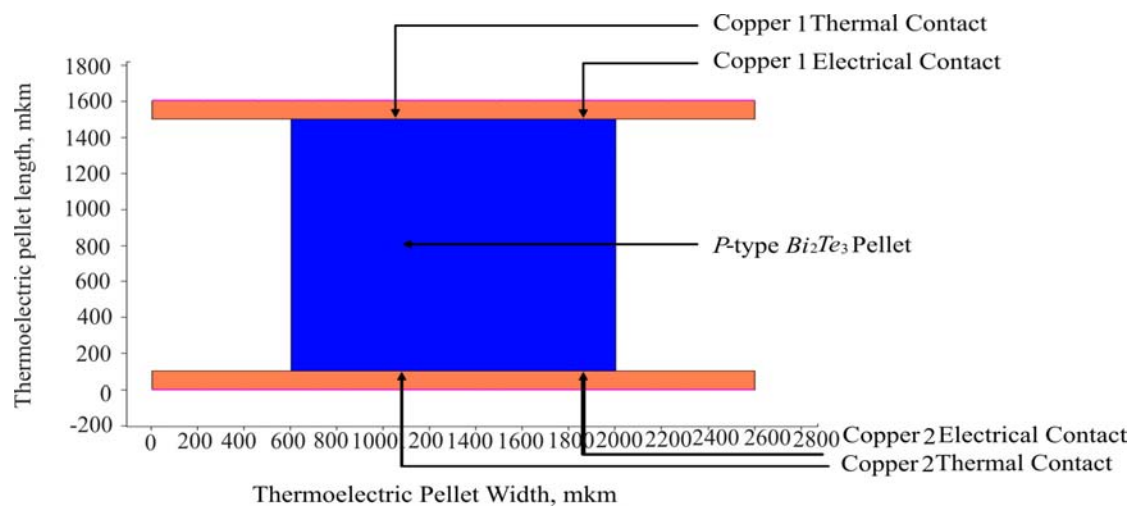

Fig. 2. p-type Bi₂Te₃ thermoelectric pellet modelled in Sentaurus Structure Editor.

Table 1

Typical material properties and dimensions of a p-type and n-type Bi₂Te₃ thermoelectric pellet at an average temperature of 300.5 K obtained from [23]

Parameter	Value	Unit	Description
α_p	215×10^{-6}	V/K	Seebeck coefficient p-type
α_n	-212×10^{6}	V/K	Seebeck coefficient n-type
ρ_p	0.00104	Ω cm	Electrical resistivity p-type
ρ_n	0.00104	Ω cm	Electrical resistivity n-type
λ_p	0.0137	W/cm K	Thermal conductivity p-type
λ_n	0.0146	W/cm·K	Thermal conductivity n-type
l_p or l_n	0.14	cm	Pellet length (p-type or n-type)
w_p or w_n	0.14	cm	Pellet width (p-type or n-type)
d_p or d_n	0.11	cm	Pellet depth (p-type or n-type)
A_p or A_n	0.0154	cm^2	Cross-sectional area(p-type or n-type)

a)
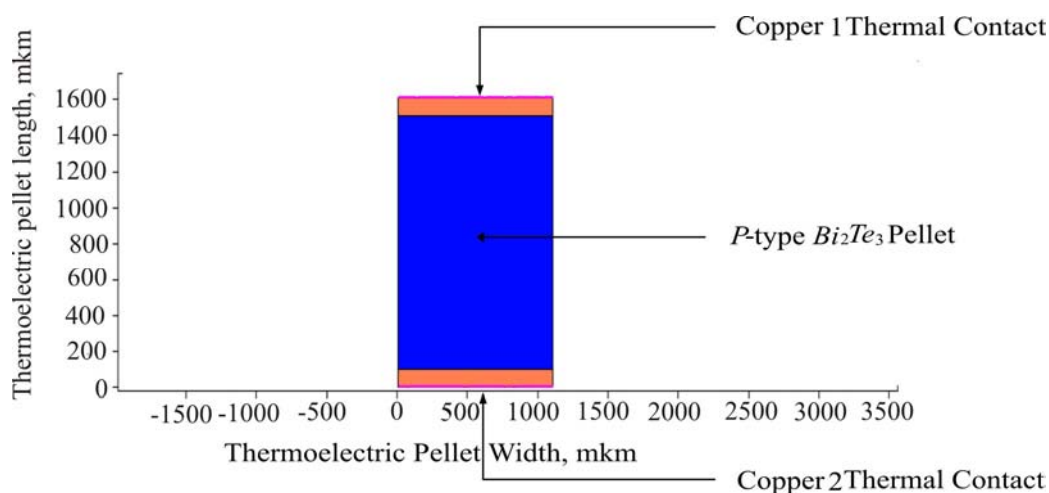
b)

Fig. 3. A cut-through in the Z-direction of the p-type Bi₂Te₃ pellet model highlighting the electrical and thermal connections (a) and a cut-through in the X-direction of the p-type Bi₂Te₃ pellet model highlighting the pellet depth in the Z-direction of 1100 micron metres (b).

<div align="right">*Table 2*</div>

Sentaurus Device (TCAD) Bi_2Te_3 thermoelectric pellet model parameters at different
average temperatures T_{avg} obtained from simulation

T_{avg} K	α_p μV	α_n μV	R_p mΩ	R_n mΩ	K_p mW	K_n mW
300.5	215	−212	9.57	9.31	1.51	1.61
312.5	222	−216	10.99	10.07	1.51	1.61
325.0	229	−220	11.01	10.90	1.51	1.61
337.5	236	−224	11.77	11.78	1.51	1.61
350.0	243	−228	12.58	12.71	1.51	1.61

Synopsys TCAD modelling and simulation of a single Bi_2Te_3 thermoelectric couple

A single Bi_2Te_3 thermoelectric couple has then been modelled in Sentaurus Structure Editor and is shown in Fig. 4(*a*). An electrode contact was made on the face of *Copper* 2 and *Copper* 3 to simulate the negative and positive electrical connections to the couple, and a thermal contact was made on the face of *Copper* 1, *Copper* 2, and *Copper* 3 in order to allow the temperature of each contact to be specified or calculated. The dimensions of the thermoelectric couple, along with the electrical and thermal contacts, are shown in Fig. 4(*b*), with the depth of the couple in the *Z*-direction equal to 1100 micron metres (1.1 mm). The simulation model is considered to be an 'ideal' representation of a thermoelectric couple, and assumes that there is no thermal resistance between the thermoelectric couple hot side T_H and the heat source, or the thermoelectric couple cold side T_C and the heat sink. Therefore, all of the heat flow between the source and sink takes place within the thermoelectric couple, and that the thermal radiation and losses by conduction and convection through the surrounding medium is considered to be negligible. The thermoelectric couple was simulated as a TCAD mixed-mode simulation, and a TCAD compact model of a load resistor R_L 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. The temperature of the thermal contact on *Copper* 1 was increased from steady state conditions of 300 K to 301 K, whilst the temperature of the other two thermal contacts, *Copper* 2 and *Copper* 3, were kept at 300 K. This creates a 1 K temperature difference between both sides of the couple. The load resistance R_L was increased from 0.001 Ωs through to 0.030 Ωs, in 0.001 Ω steps, in order to establish where maximum power transfer occurs. The voltage V_L and current I_L at the load was recorded using the simulation program, and the electrical power generated at the load calculated using the equation $P_L = V_L \times I_L$. The electrical power generated at the load is shown in Fig. 5 and reaches a peak value of 2.61 μW with a load resistance of 0.017 Ωs, where maximum power transfer is observed.

The couple was then tested with the temperature of the thermal contact on *Copper* 1 increased from 301 K to; 325 K; 350 K; 375 K; and 400 K. The temperature of the other two thermal contacts, *Copper* 2 and *Copper* 3, were kept at 300 K. This creates a temperature difference between both sides of the couple of; 25 K; 50 K; 75 K; and 100 K respectively. The power generated at the load, shown in Fig. 6, can be seen to increase as the temperature gradient increases, and peaks at 22.67 mW with a load resistance of 0.025 Ωs and a temperature of 400 K applied to the thermal contact *Copper* 1 located at the top of the device.
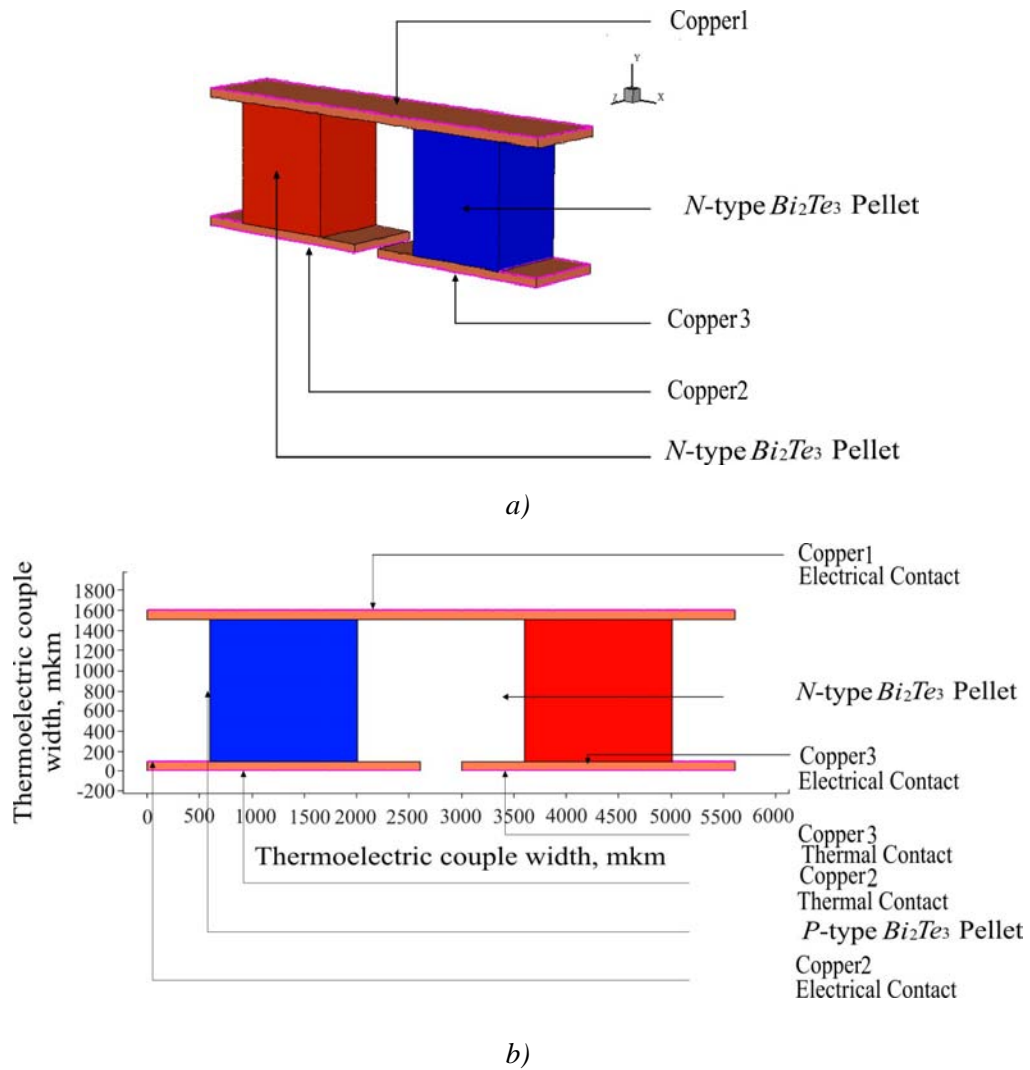
a)

b)

Fig. 4. A Bi$_2$Te$_3$ thermoelectric couple modelled in Sentaurus Structure Editor (a)
and a cut-through in the Z-direction of the Bi$_2$Te$_3$ thermoelectric couple model
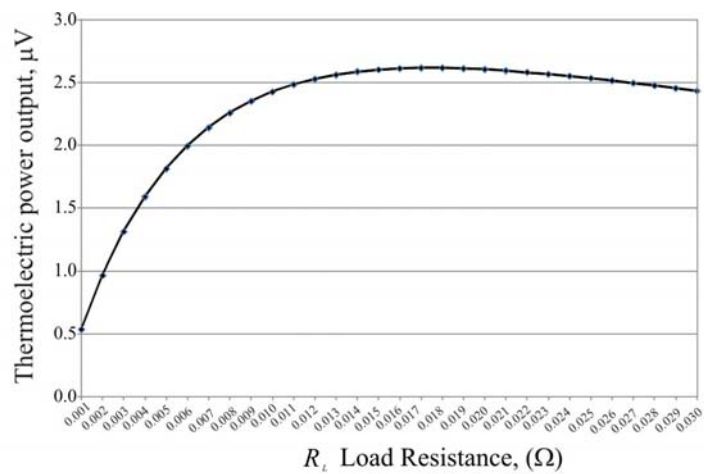*highlighting the electrical and thermal connections (b).*

Fig. 5. The thermoelectric output power generated at the load when the Bi$_2$Te$_3$ thermoelectric
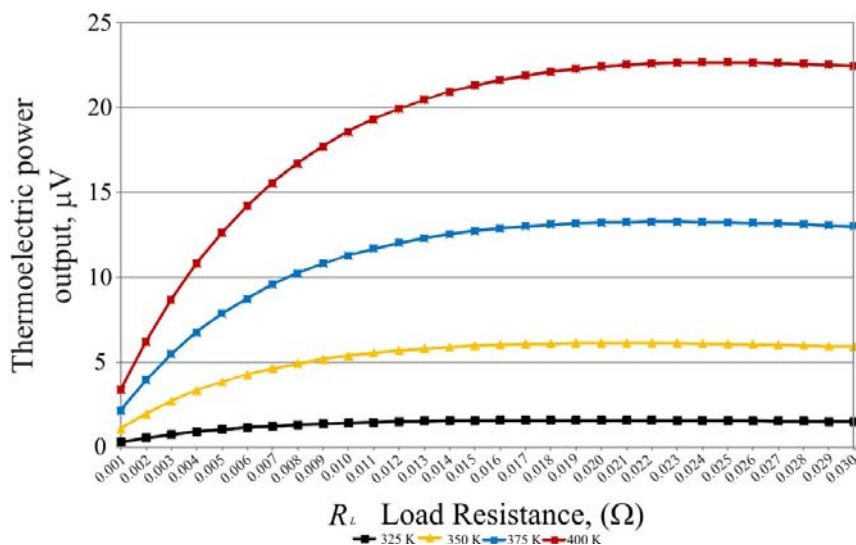*couple is subjected to a 1 K temperature gradient (Simulation result).*

Fig. 6. The thermoelectric power generated at the load when the thermal contact
Copper 1 located at the top of the device is set to 325, 350, 375, and 400 K,
creating a temperature gradient of 25, 50, 75 and 100 K respectively across
the device (Simulation result).

Numerical analysis of a single *Bi₂Te₃* thermoelectric couple

In order to validate the TCAD simulation results, an analysis can be made to compare the simulation results obtained in TCAD, which uses in-built semiconductor physics equations that calculate, amongst others, the; electrostatic potential; thermodynamic carrier transport; the lattice, electron, and hole temperatures; and the electron and hole absolute thermoelectric powers; with the results obtained by numerical calculation using a different set of equations published in thermoelectric literature that describes the behaviour of a single thermoelectric couple when it is subjected to a temperature gradient. According to [24], if we consider that no other heat arrives at the cold side T_c other than through the two thermoelectric legs, the thermoelectric couple open-circuit voltage V_{oc} can be found by:

$$V_{oc} = \left(\alpha_p - \alpha_n \right)\left(T_h - T_c \right) \quad , \tag{8}$$

where α_p and α_n is the Seebeck coefficient of the *p*-type and *n*-type pellets of the thermoelectric couple respectively, T_h is the surface temperature of the hot side of the thermoelectric couple, and T_c is the surface temperature of the cold side of the thermoelectric couple, measured in K. The electrical resistivity ρ of each pellet can be found and/or measured, and the resistance R_p of the *p*-type pellet can then be calculated using:

$$R_p = \frac{L_p \, \rho_p}{A_p} \quad , \tag{9}$$

where ρ_p is the electrical resistivity of the pellet in Ωs/cm, L_p is the length of the pellet in cm, and A_p is the cross-sectional area of the pellet in cm^2 found by:

$$A_p = \text{width} \times \text{depth} . \tag{10}$$

Similarly, the resistance of the *n*-type pellet R_n can be found. The thermoelectric couple resistance R_c, ignoring the resistance of the copper interconnects, is the addition of the resistance of the two thermoelectric pellets:

$$R_c = R_p + R_n .$$ (11)

The resistance of the copper interconnects is typically in the mΩ region, and compared with the resistance of the *Bi$_2$Te$_3$* thermoelectric pellets, which tends to be in the milli ohm region, is significantly smaller in value and hence can be considered as negligible. The thermal conductivity λ of each pellet can be found and/or measured, and the thermal conductivity K_p of the *p*-type thermoelement calculated by:

$$K_p = \frac{\lambda_p A_p}{L_p} ,$$ (12)

where λ_p is the thermal conductivity of the pellet in W/cm·K, L_p is the length of the pellet in cm, and A_p is the cross-sectional area of the pellet in cm^2. Similarly, the thermal conductivity of the *n*-type pellet K_n can be found. The current *I* can be expressed as:

$$I = \frac{V}{R_T} ,$$ (13)

where *V* is the closed-circuit voltage, and R_T is the total resistance of the thermoelectric couple and the load. It is possible to find R_T using:

$$R_T = R_p + R_n + R_L .$$ (14)

As the load resistor R_L is connected across the output terminals of the couple, the load current I_L is the same as the circuit current *I,* and the voltage generated at the load V_L can be found by:

$$V_L = I_L \times R_L .$$ (15)

the electrical power generated at the load can be found by:

$$P_L = V_L \times I_L$$ (16)

The efficiency η of a thermoelectric couple can be found by:

$$\eta = \frac{\text{Energy supplied to the load}}{\text{Heat energy absorbed at the hot junction}} .$$ (17)

The electrical power supplied to the load is P_L, and according to [24], the cooling power at the hot side of the thermoelectric couple Q_h can be found by:

$$Q_h = \left(\alpha_p - \alpha_n \right) I T_h - \left(T_c - T_h \right) \left(K_p + K_n \right) - \frac{I^2 \left(R_p + R_n \right)}{2}$$ (18)

Hence, the efficiency of the thermoelectric couple η can now be found by equation (17), and written as:

$$\eta = \frac{P_L}{Q_h} .$$ (19)

In thermoelectricity, efficiency is expressed as the dimensionless figure-of-merit Z, or more commonly, expressed as a function of the temperature over which the device is operated Z_T, which can be found by:

$$Z_T = \frac{\alpha^2 \sigma}{\lambda},$$ (20)

where α is the Seebeck coefficient, σ is the electrical conductivity, and λ is the thermal conductivity of the couple at a specific operating temperature. The Bi_2Te_3 thermoelectric couple TCAD simulation results have been summarised in Table 3 for ease of comparison, and demonstrate good agreement between the expected result obtained by numerical calculation using equations (8 – 20), and the results obtained by TCAD simulation that uses a different set of in-built semiconductor equations that include, amongst others, equations (1 – 7).

Table 3

A summary of the Bi_2Te_3 thermoelectric couple TCAD simulation results

	T_H K	T_C K	ΔT K	V_{oc} mV	I_L mA	V_L mV	P_L mW	R_L Ω	Efficiency η %	Z_T
Calculated	301	300	1	0.427	11.31	0.21	0.00242	0.019	0.05	3.10×10^{-3}
TCAD	301	300	1	0.427	12.41	0.21	0.00262	0.017	0.06	3.44×10^{-3}
Calculated	325	300	25	10.95	260	5.48	1.42	0.021	1.25	2.77×10^{-3}
TCAD	325	300	25	10.96	289	5.49	1.59	0.019	1.36	2.78×10^{-3}
Calculated	350	300	50	22.45	512	11.23	5.75	0.022	2.50	2.67×10^{-3}
TCAD	350	300	50	22.49	540	11.35	6.13	0.021	2.63	2.67×10^{-3}
Calculated	375	300	75	34.50	733	17.25	12.64	0.024	3.67	2.48×10^{-3}
TCAD	375	300	75	34.50	760	17.48	13.20	0.023	3.78	2.48×10^{-3}
Calculated	400	300	100	47.10	931	23.55	21.93	0.025	4.77	2.31×10^{-3}
TCAD	400	300	100	47.04	952	23.80	22.67	0.025	4.90	2.31×10^{-3}

Synopsys TCAD simulation of a Bi_2Te_3 thermoelectric couple with ceramic outer plates

A single thermoelectric couple with ceramic outer plates of thermal conductivity 0.3 W/cm·K has been simulated, shown in Fig. 7(*a*) and Fig. 7(*b*). The top and bottom faces 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 for a single thermoelectric couple without ceramic outer plates. If the top of the device, where the thermal contact *Ceramic Top* is located, is set to 301 K, and the thermal contact *Ceramic Bottom* is maintained at 300 K, creating a 1 K temperature gradient, the electrical power generated at the load peaks at 2.48 mW with a load resistance of 0.017 Ωs, which is slightly lower than the 2.61 mW obtained without the ceramic outer plates. The ceramic outer plates absorb heat energy changing the temperature gradient, and the temperature gradient within the thermoelectric pellet has been reduced, resulting in less electrical power generated at the load. However, the ceramic plates are necessary in practical devices in order to create electrical isolation and provide a foundation to mount the thermoelectric couple. Further simulations have been performed with a temperature difference between both sides of the couple of; 25 K; 50 K; 75 K; and 100 K respectively, with the power generated at the load shown in Fig. 8. The electrical power generated at the load peaks at 21.50 mW with a load resistance of 0.025 Ωs, and a temperature gradient of 100 K maintained across the couple.
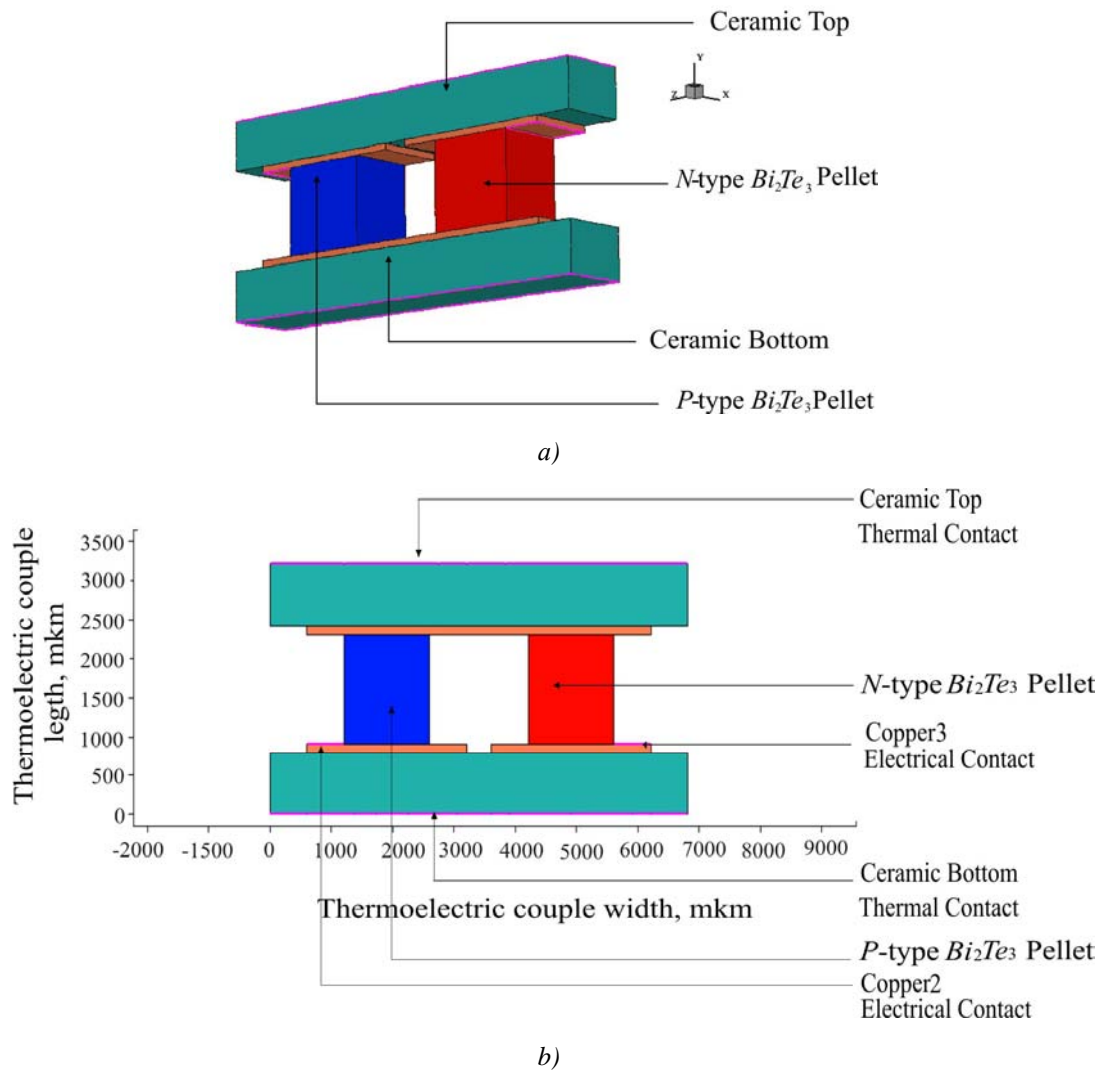
a)

b)

Fig. 7. A Bi₂Te₃ thermoelectric couple with ceramic outer plates modelled in Sentaurus Structure Editor (a) and a cut-through in the Z-direction, highlighting the electrical and thermal contacts (b).
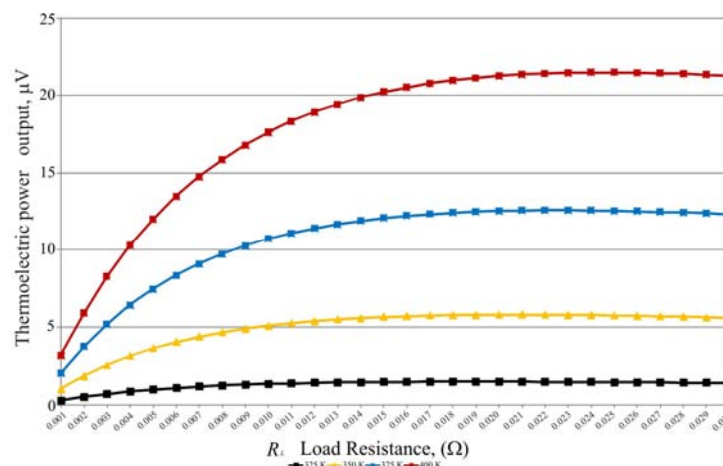

Fig. 8. The thermoelectric power generated at the load when the thermal contact Ceramic Top is set to 325 K, 350 K, 375 K, and 400 K, creating a temperature gradient of 25, 50, 75 and 100 K respectively across the device (Simulation result).

Synopsys TCAD modelling and simulation of a seven couple *Bi₂Te₃* thermoelectric module

A seven couple *Bi₂Te₃* thermoelectric module with ceramic outer plates has also been successfully modelled and simulated, and is shown in Fig. 9 through to Fig. 11. The top and bottom faces of the two ceramic plates have been used as the thermal contacts of the device, and are labelled *Ceramic Top* and *Ceramic Bottom* respectively. When the temperature of the thermal contact *Ceramic Top* is set to 301 K, and the temperature of the thermal contact *Ceramic Bottom* is set to 300 K, creating a one K temperature gradient, the electrical power generated at the load peaks at 19.2 µW with a load resistance of 0.11 Ωs. If we compare this with the power output for a single *Bi₂Te₃* thermoelectric couple with ceramic outer plates, the electrical power generated at the load was 2.48 µW with a load resistance of 0.017 Ωs. The seven couple *Bi₂Te₃* module generates over seven times as much power as the single thermoelectric couple model. This is as expected as the voltage output of each couple due to the Seebeck effect is connected electrically in series to one another, and hence the total voltage output will be the summation of each of the individual couples output. The resistance of the seven couple thermoelectric module has also increased approximately seven times, and is in-line with expectations.
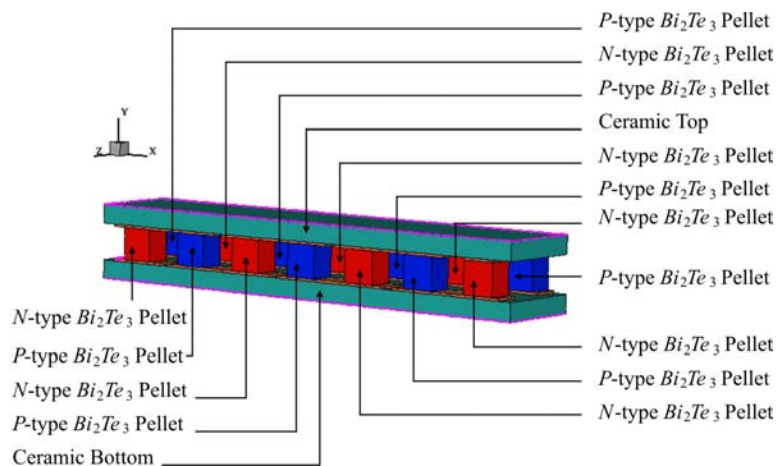

Fig. 9. A seven couple Bi₂Te₃ thermoelectric module with ceramic outer plates
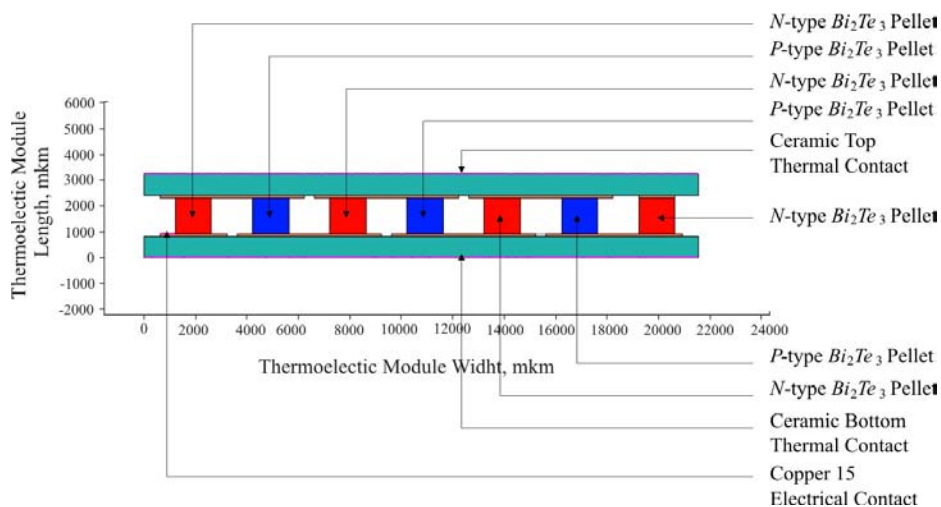*modelled in Sentaurus Structure Editor*

Fig. 10. A cut-through in the Z-direction of the seven couple Bi₂Te₃ thermoelectric
module, highlighting the electrical and thermal contacts on one side of the module.
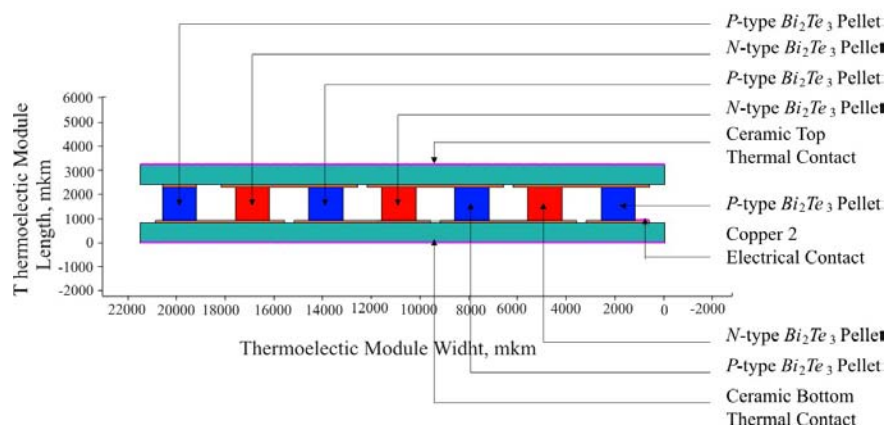
*Fig. 11. A cut-through in the Z-direction of the seven couple Bi$_2$Te$_3$ thermoelectric
module, highlighting the electrical and thermal contacts on the other side of the module.*

Increasing the temperature gradient across the seven couple *Bi$_2$Te$_3$* module, shown in Fig. 12, results in an increase in electrical power generated at the load as expected. The seven couple *Bi$_2$Te$_3$* thermoelectric module now generates 162.17 mW at 0.16 Ωs with a temperature gradient of 100 K.
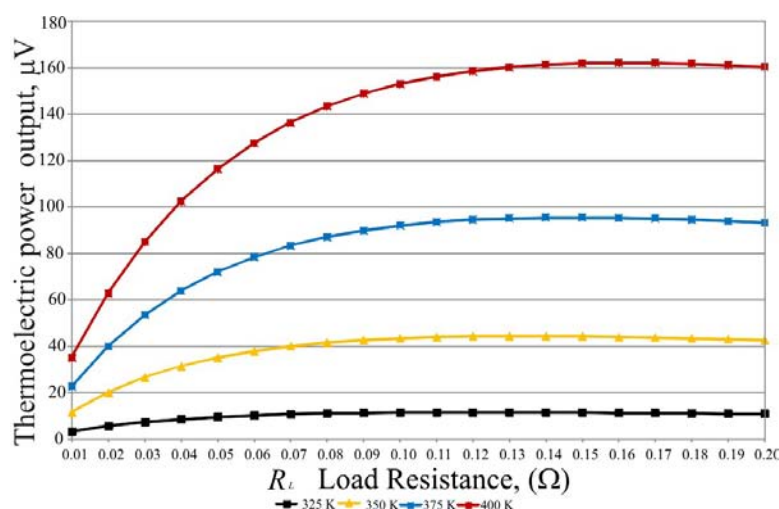

*Fig. 12. - The thermoelectric power generated at the load when the thermal contact
Ceramic Top is set to 325, 350, 375, and 400 K, creating a temperature gradient
of 25, 50, 75 and 100 K respectively across the device (Simulation result).*

Discussion

The aim of this work has been to develop Synopsys TCAD simulation models of a Bismuth Telluride (*Bi$_2$Te$_3$*) thermoelectric couple and a seven couple thermoelectric module. This has been successfully achieved and the TCAD simulation models demonstrate very good correlation with expected behaviour and theory. Focusing on the single *Bi$_2$Te$_3$* thermoelectric couple simulation model, when the couple is subjected to a temperature gradient, a small amount of electrical power is generated at the load. This is in-line with expected behaviour, and a comparison between the results obtained in the TCAD simulation, which are based on the simulation programs use of in-built semiconductor physics models and equations that calculate, amongst others, the; electrostatic potential; thermodynamic carrier transport; the lattice, electron, and hole temperatures; and the electron and hole absolute thermoelectric powers; with the results obtained by numerical calculation using a different set of equations published in thermoelectric literature are in close agreement.

Similarly, the simulation model highlights that the amount of electrical power generated at the load is dependent on the level of temperature difference that exists between both sides of the couple. It can be demonstrated that a 100 K temperature difference across the couple generates far more electrical power at the load than can be observed with a 1 K temperature difference. Again, this is as expected, as the Seebeck effect, which has the most influence in thermoelectric power generation, is temperature dependent. The development of a single Bi_2Te_3 thermoelectric couple with ceramic outer plates highlights that the ceramic plates absorb heat energy changing the temperature gradient, resulting in the temperature gradient within the thermoelectric pellets reducing, and slightly less electrical power is generated at the load when compared to the thermoelectric couple without ceramic outer plates. However, the ceramic plates are necessary to create electrical isolation and provide a foundation to mount the thermoelectric couple. The TCAD seven couple Bi_2Te_3 thermoelectric module simulation results correctly demonstrate that by connecting several thermoelectric couples together electrically in series, and thermally in parallel, the module will generate approximately seven times more electrical power at the load than can be obtained from a single Bi_2Te_3 thermoelectric couple.

This is in-line with expected behaviour and, similar to the single Bi_2Te_3 thermoelectric couple model, a comparison between the results obtained in the TCAD simulation with the results obtained through numerical calculation by applying a different set of theoretical equations is in close agreement. Future work will provide further validation of the TCAD simulation results with practical test samples. A seven couple Bi_2Te_3 thermoelectric module was developed in Synopsys TCAD as this size of module is relatively straightforward for a thermoelectric manufacturer to produce, and test samples with the same dimensions and material properties used in the TCAD simulation model will be manufactured and subjected to the same test methodology. In this way, the Synopsys TCAD simulation results can be triangulated with the results obtained from testing a physical thermoelectric module and by calculated theory, with a full set of test results published.

Employing Synopsys TCAD to model and simulate thermoelectric generators has several advantages. It is an ideal platform to rapidly design, model, and simulate the behaviour of novel thermoelectric device structures and materials at a range of different temperature gradients, including the next generation of thermoelectric modules based on thin-film and nanotechnology. The simulation package is extensively used in the wider electronics semiconductor industry to model and simulate the behaviour of VLSI devices, and can support very small device geometry sizes. When a thermoelectric material has been defined in the materials database, in this case Bi_2Te_3, and a one, two, or three dimensional thermoelectric device structure is created, a series of simulations can be automatically executed at different temperatures of interest, and TCAD will calculate the key thermoelectric parameters, including the Seebeck coefficient, as the program executes each discrete temperature step. Furthermore, it is possible to model and simulate a thermoelectric couple or module as a single device, or as a mixed mode simulation, where the thermoelectric device can be connected to external components, for example, a load resistor or capacitor connected across the thermoelectric module's output terminals, or several different thermoelectric modules that have been designed in TCAD can be connected together in series or in parallel as part of a system. It is also possible to set-up a relatively complex simulation strategy that automatically modifies key variables in order to obtain a series of simulation results at different set-points. An additional capability within Synopsys TCAD is the ability to model and simulate the semiconductor manufacturing process, i.e. deposition, diffusion, and photolithography, which can be integrated with the TCAD device modelling and simulation tool sets. Future work will investigate

applying TCAD's semiconductor process simulation capability to thermoelectric devices and the results will be published.

Conclusions

A single *Bi$_2$Te$_3$* thermoelectric couple, and a seven couple *Bi$_2$Te$_3$* thermoelectric module, have been successfully modelled and simulated in Synopsys TCAD semiconductor design and simulation software. The simulation results obtained for thermoelectric power generation are in agreement with expected behaviour, with the model correctly demonstrating that when a temperature gradient is applied to a thermoelectric device, electrical power is generated at the load due to the Seebeck effect, with the amount of generated power dependent on the level of temperature gradient that exists across the device. It can also be observed that by connecting several thermoelectric couples together electrically in series, and thermally in parallel, a thermoelectric module will generate higher levels of electrical power at the load than can be obtained from a single thermoelectric couple. A comparison between the results obtained in the TCAD simulation, which are based on the simulation programs use of in-built semiconductor physics models and equations, and that obtained by applying a different set of thermoelectric equations, are also in close agreement and can be used to validate the simulation results. The Synopsys TCAD thermoelectric model can be developed in the future to investigate the effect of different thermoelectric device structures, and will enable new thermoelectric materials to be investigated, within the framework of the simulation environment, in an attempt to improve the performance, efficiency, and cost of thermoelectric devices.

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