Modelling of a Thin Film Thermoelectric Micro-Peltier Module

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ABSTRACT

A micro Peltier cooler/heater module has been modelled. The module consists of n-type bismuth telluride and p-type antimony telluride thermoelectric materials. The commercial software package CFD-ACE+ has been used to implement and analyse the model. A two-dimensional coupled electrical and thermal simulation was performed. This software includes the possibility to incorporate the Peltier effect. The temperature, electric field intensity and wall heat flux distributions were simulated for different applied potentials. The variation in temperature difference with respect to the Seebeck coefficient of the material was calculated and analysed.

1. INTRODUCTION

Peltier thermoelectric modules are widely used in microelectronics for temperature control and stabilization [1]. There is an increasing demand in the applications of thermoelectrics for the semiconductor and optical communication industry [2] [3]. Microprocessors, micro–sensors, micro-controllers and lab-on-a-chip are among some of the devices, which require an efficient temperature control during their operation. A conventional thermoelectric cooler consists of a number of n- and p-type semiconductors, which are electrically in series but thermally in parallel. The functionality of such devices is based on the bulk property of the materials [4]. Thus these devices are incompatible with microelectronic fabrication processes. Thin film micro-thermoelectric modules offer higher efficiency than their bulk counterparts due to quantum and classical size effects of electrons and phonons [5]. However to date, such thin film thermoelectric Peltier modules have not been successfully used in commercial micro cooler/heater applications. The technological practicality of thermoelectric cooling is by and large constrained by the poor performance factor. This could be due to the large dependence on the properties of the materials used in these devices. The main benefit of using thin film technology is the dramatic increase in the cooling power density [6].

Prospects of optimising the geometrical dimensions and the design parameters to achieve higher performance could be achieved through modelling of the specified device. The multi-physics simulation software from CFD Research Corporation (*http://www.cfdrc.com*) provides a useful tool for the design and simulation of the micro Peltier modules. This software is an advanced multi-physics package for modelling thermal and electrical effects in individual semiconductor devices, packages, boards, and complete electronic enclosures. The software has the ability to run parametric studies, which significantly help to achieve optimization of the device design.

In this paper, we modelled a micro Peltier module consisting of one n-type and one p-type semiconductor. The modelled device has been investigated based on material properties and for different temperatures. Furthermore, the temperature, electric field intensity and wall heat flux distributions were studies.

2. THEORY

N-type semiconductor bismuth telluride (Bi_2Te_3) and p-type semiconductor antimony telluride (Sb_2Te_3) are widely used low operational temperature materials for the development of Peltier cooler/heater modules [4]. These materials have a high Seebeck coefficient, moderate electrical conductivity and low thermal conductivity. As a result, they have a high figure of merit, which is a significant factor for the improvement of efficiency of the micro Peltier modules.

Figure of merit is defined as:

$$Z_{p,n} = \frac{S_{p,n}^{\;2}}{\rho_{p,n}\,\lambda_{p,n}} \tag{1}$$

where $S_{p,n}$ is the Seebeck coefficient of the material (μV/K), $\rho_{p,n}$ is the electrical resistivity (μΩm) and $\lambda_{p,n}$ is the thermal conductivity (W/m-k).

The suffix *n* & *p* denotes the respective material properties for the n- and p-type semiconductors employed. $\rho_{p,n}$ and $\lambda_{p,n}$ depend on the geometrical parameters of cross-sectional area (*A*) and the length (*L*) of the semiconductor component.

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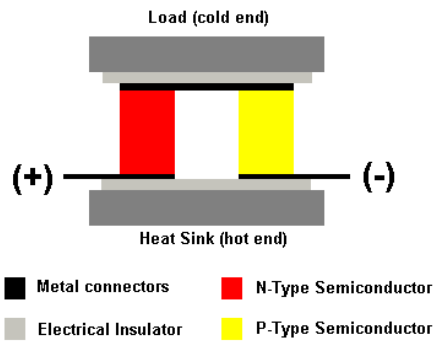


Figure 1: Schematic diagram of a thermoelectric Peltier module

The thermoelectric micro Peltier module used in the simulation is shown in Figure 1. It consists of the n- and p-type thermoelectric materials sandwiched between two electrical insulators. The cold end carries the heat load, thereby creating a temperature difference across the device. As a result of this temperature difference, a heat flux appears. The heat is transferred from the load (cold end) to the heat sink (hot end) via conduction, since the materials are in physical contact with each other. It takes place at the molecular level and involves the transfer of energy from the higher energetic molecules to those at a lower energy level [7].

The change in temperature ΔT can be expressed as a function of the material parameters [4], such as

$$\Delta T = \frac{1}{2} Z_{p,n} T_c^{\,2} \qquad (2)$$

where T_c is the temperature in Kelvin at the cold surface.

From equations 1 and 2, it is clear that the figure of merit $Z_{p,n}$, the change in temperature ΔT and the geometrical dimensions (A and L) of the device are all inter dependent. Therefore to simplify the design parameters in the simulation of the micro Peltier module, the material properties and the dimensions of the device were kept constant.

3. SIMULATION

The coupled heat and electrical analysis was performed for a two dimensional micro Peltier module. The simulations provided a means to observe the variation in temperature across the device. The simulated model consists of a cross-sectional area (A) and leg length (L) of 10 μm^2 and 1μm, respectively. Silicon Carbide (SiC) was used as the electrical insulator and heat sink element because of its high thermal conductivity. The thickness of SiC employed was 1 μm. it was placed above the electrical connector and under the pads to provide efficient electrical isolation and higher rate of thermal transfer. A 0.25 μm thick aluminium layers provide electric connection between the two semiconductors and the voltage source. The distance between the two semiconductors was 5 μm. The material properties [8] are listed in Table 1.

Table 1 Properties of the materials used in the simulation

Material Properties	***Bi_2Te_3***	***Sb_2Te_3***	***Al***	***SiC***
Density (kg/m^3)	7700	6500	2700	3210
Specific Heat Capacity (J/kg-K)	155	210	900	750
Thermal Conductivity (W/m-K)	1	1	240	120
Electrical Resistivity (Ωm)	$1x10^{-5}$	$1x10^{-5}$	$5x10^{-9}$	$1x10^{4}$
Seebeck coefficient (μV/K)	-230	180	3.5	-10

Figure 2 shows the structured mesh used in the simulation. Approximately 30,000 nodes were generated after meshing. Up to 4 nodes for a length of 0.25μm was used. The mesh has the same shape and size in al the components of the module.

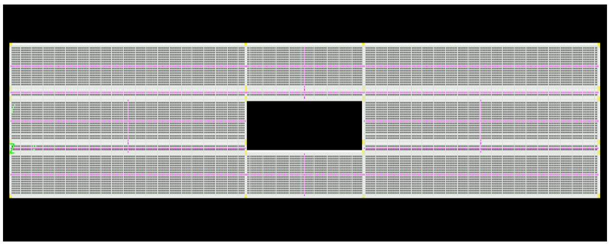


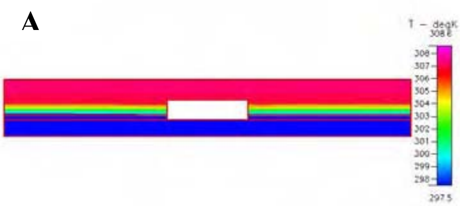
Figure 2: Two-dimensional mesh format for the micro Peltier module

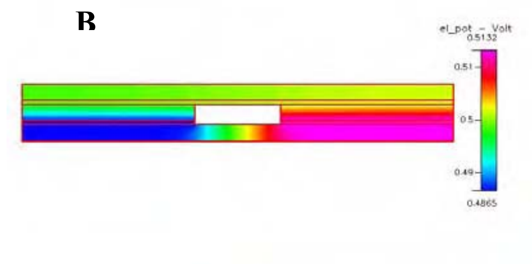
The geometrical parameters used in the simulation were assumed to be constant throughout the simulation. This assumption was carried out in order to study the effect of the material properties on the device performance as a function of change in temperature. The effect of change in Seebeck coefficient of the semiconductor materials for similar dimensions of both the n- and p-type materials was investigated. The length of the semiconductor blocks were ($L=L_p=L_n$) 1μm each and the cross-sectional area ($A=A_p=A_n$) was 10 μm^2. This model is based on the assumption that the heat transfer mechanism across the device is purely conduction. The boundary condition on the sidewalls was assumed to be adiabatic.

All the simulations were conducted with constant electrical current and the temperatures were fixed at both the hot and the cold end. Normally these are the reference conditions provided by the commercial manufacturers [9]. A number of simulations were performed, corresponding to different changes in temperature between the hot and the cold end. The deviation in the temperature difference was in the range of 1 to 10 K. A 38.5 mV voltage was applied across the Peltier module and the temperature, electric field intensity and wall heat flux distributions were simulated. They are shown in Figure 3. As can be seen, a heat flux is generated due to the Peltier effect. The module is capable of generating approximately 40K localized temperature difference. A current of 0.1 A was passing through the module at this voltage. There was a quasi-linear electric field distribution in the two semi-conductors.

In order to observe the Peltier effect, a series of simulations were performed for different values of the Seebeck coefficient for Bi_2Te_3 while the coefficient was kept constat for Sb_2Te_3 at 180 μV/K. They were changed in the range of –140 to –250 μV/K and the temperature differences were calculated. Figure 4 shows comparison of change in temperature calculated from equation (2) to the simulated one based on the material properties of the semiconductors. The properties of the materials were found to largely influence the performance of the micro Peltier module. As can be seen for the average values of the Seebeck coefficients greater than 180μV/K only an appreciable temperature difference was observed. However the temperature difference obtained for the numerical calculations was found to be linear.

Although the dimensions of the semiconductor components were the same, there are some discrepancies in the distribution of the of electric field intensity. This could be attributed due to the mismatch of the Seebeck coefficients of different materials in the thermoelectric micro Peltier module. Arenas et al [9] reported similar discrepancies. In addition the difference in the calculated and simulated values could be due to some of the assumptions related to heat transfer mechanisms.





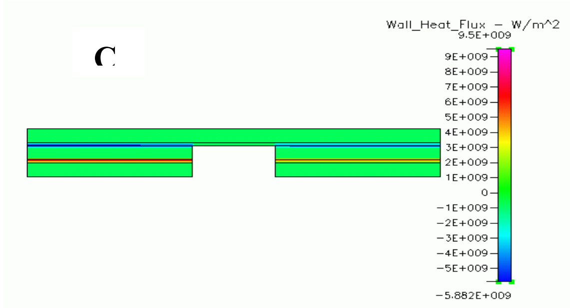


Figure 3 Distribution of A) temperature, B) electric field intensity and C) wall heat flux

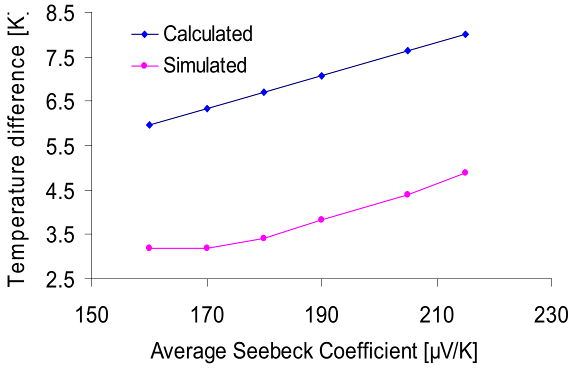


Figure 4: Temperature difference versus the average magnitude of the Seebeck coefficient of semiconductor materials

4. CONCLUSION

A two- dimensional simulation for a single pair n- and p-type thermoelectric micro Peltier module has been performed. The commercial software package CFD-ACE+ has been used. At 38.5 mV, 0.1 A current was drawn by the module and a temperature change of 40.5K was observed. The temperature, electric field intensity and wall heat flux distributions were analysed. Simulations for different Seebeck coefficients for the thermoelectric materials have been conducted. Significant variations in the performance of the device were observed. The simulation approach using the software package CFD-ACE+ offers an efficient solution for modelling micro-Peltier modules. A 3D simulation is planned for the next modelling stage. Additionally, the effect of variation of the semiconductor material thickness on the module performance will be investigated.

5. ACKNOWLEDGEMENT

The authors would like to thank CASS Foundation, Australia for providing financial support for this project.

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