Asymmetry Induced Terminal Voltage Improvement in Mg_2Si-based Thermoelectric Unicouple

Pankaj Priyadarshi[1], Jyotsna Bahl[2], and Bhaskaran Muralidharan*[1]
[1]Department of Electrical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai
[2]Centre for Research in Nanotechnology and Science, Indian Institute of Technology Bombay
*bm@ee.iitb.ac.in

Abstract: In this work, we propose the incorporation of asymmetry in Mg_2Si-based thermoelectric unicouple element primarily to enhance the output voltage of thermoelectric generator. Asymmetrical shape of thermoelectric leg helps in two-ways, a) harnessing the Thomson effect, which depends on the temperature gradient in the leg and temperature variation of Seebeck coefficient of the material as the operating temperature range, and is generally neglected in conventional rectangular thermoelements, b) reducing the overall electrical resistance of the device. Mg_2Si-based alloys are promising medium range thermoelectric materials and selected for the current application due to their larger variation in Seebeck coefficient with temperature as compared to conventional Bi_2Te_3 based thermoelectrics. Finite element simulation in COMSOL Multiphysics has been performed on different geometries of thermoelectric unicouple and finally, it has been found that increasing the tapering factor or thickness of a p-leg increases the output terminal voltage and hence efficiency of the thermoelectric unicouple module depending upon the load resistance and dimensions of the device.

Keywords: Thermoelectric unicouple, Seebeck effect, Tapered leg

1. Introduction

In the light of issues of global warming, thermoelectricity is the most challenging technology as a candidate of clean energy sources. Due to its noiseless, low-cost operation and maintenance, it has a great impact as the conventional thermal to electric power generation have. The effect of thermoelectricity includes mainly three coupled effects:- Seebeck, Peltier and Thomson Effect [1]. However, the efficiency of a thermoelectric device is largely described in terms of extrinsic parameters such as hot and cold side temperature, length & crossectional area of thermoelectric leg, and load resistance [2].

Over the many decades, a thermodynamic theory has been developed to model the thermoelectric devices, preliminary coupled equations in matrix form needed to solve the thermoelectric device problem is:-

$$\begin{bmatrix} J \\ J_Q \end{bmatrix} = \begin{bmatrix} \sigma & \alpha\sigma \\ T\alpha\sigma & \kappa \end{bmatrix} \begin{bmatrix} E \\ -\nabla T \end{bmatrix} \qquad (1)$$

where, α, σ and κ are the material parameteres- Seebeck coefficient, electrical conductivity and thermal conductivity respectively. J is the electrical current density, J_Q heat flux density, E electric field and T temperature.

Although one can deduce the terminal voltage across the unicouple by averaging the Seebeck coefficient over the temperature ranges i.e. from hot to cold end. The terminal voltage V_{oc} for a rectangular leg could be calculated by:

$$V_{oc} = \int_{T_C}^{T_H} \alpha(T)\, dT \qquad (2)$$

The above equation can be derived from the coupled equations as given by [3]. But apart from the averaging Seebeck coefficient, thermal and electrical resistance also play a key role in defining the terminal electrical voltages on the account of temperature differences [4]. These explanations can be included with varying electrical as well as thermal resistance along with the length of thermoelectric legs shown in figure 1, as following expressions:-

Electrical Resistance,

$$R = \int dR = \frac{1}{\sigma} \int \frac{dx}{wy} \qquad (3)$$

Thermal Conductance,

$$K = \int dK = \kappa_{avg} \int \frac{wy}{dx} \qquad (4)$$

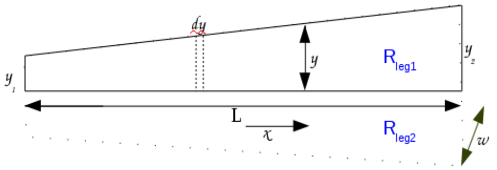

Figure 1. Trapezoidal varying of crossectional area of the thermoelectric legs along the length.

Here, L is length of the leg, w is width of the leg and y, the varying thickness along the length. Thus, the overall output terminal voltage can be calculated as:

$$V_{out}=V_{oc}\frac{R_{Load}}{R_{inte}+R_{Load}} \tag{5}$$

Where, R_{inte} include the effect of geometry of the legs to account for electrical and thermal resistance.

2. Simulation Setup

Finite element simulations on 2D-axisymmetric and 3D geometries of the Mg_2Si-based thermoelectric unicouple using the dedicated "Thermoelectric module of COMSOL Multiphysics" for a theoretical analysis of temperature profile, heat flux in the presence of asymmetry, and the terminal voltage has been carried out. Heat balance equation solved in COMSOL Multiphysics for the thermoelctric effect [5] is:

$$\rho C_p\frac{\partial T}{\partial t}+\nabla\left(-\kappa\nabla T+PJ\right)=Q \tag{6}$$

In the above equations, ρ is the density of material, C_p the specific heat at constant pressure, P the Peltier coefficient and Q the extrinsic heat source. For the steady state solution, $\partial T/\partial t = 0$. A thermoelectric effect node also adds the term '$-\sigma\alpha\nabla T$' to the current density, which is then defined as:

$$J=-\sigma\left(\nabla V+\alpha\nabla T\right) \tag{7}$$

where, σ is the electrical conductivity of the material. In this simulation process, the electrical current density is treated as uniform throughout the device. Temperature dependent material properties like Seebeck coefficient, thermal conductivity and electrical conductivity of Mg_2Si-based alloys (p-type $Mg_2Si_{0.6}Ge_{0.4}$: Ga-0.8% and n-type $Mg_2Si_{0.3}Sn_{0.7}$) have been taken from literature [6, 7], shown in figure 2, 3 and 4.

p-n unicouple geometry

A schematic of p-n unicouple used for simulations is shown in figure 5. The dimensions are:

a) Leg: 2.15*mm* x 2.98*mm* x 6.22*mm*
b) Copper plates (both end): 2.15*mm* x 2.98*mm* x 0.5*mm*
c) Distance between legs: 1.0*mm*

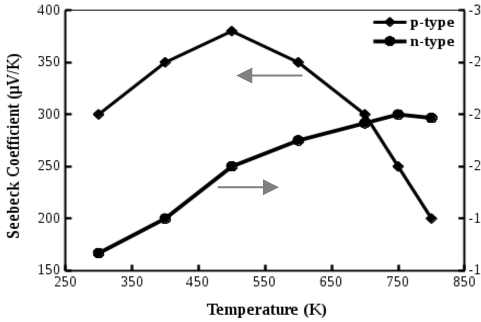

Figure 2. Seebeck coefficient of p- & n-type Mg_2Si based material varying with temperature (300–800 K)

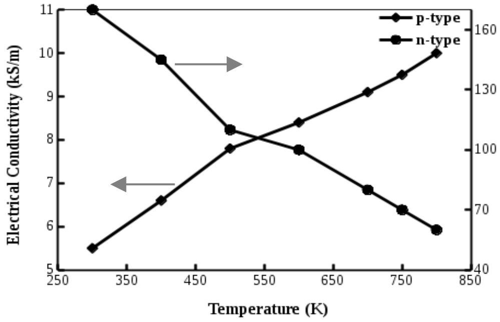

Figure 3. Electrical conductivity of p- & n-type Mg_2Si based material varying with temperature (300–800 K)

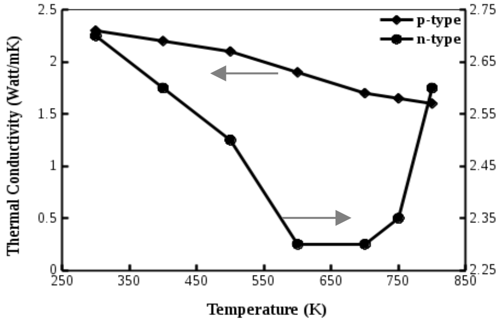

Figure 4. Thermal conductivity of p- & n-type Mg_2Si based material varying with temperature (300–800 K)

One end of the couple is kept at 296.55 K while another end at 420.75 K. The end of right side n-leg, shown in figure 5 (a to f) is grounded and current is applied from left end towards p-side. A current of 0 *A* to 2.0 *A* is applied to the terminal and changes in potential generated is studied for different geometries and shapes of thermoelectric legs. A tapering factor is introduced which signifies the ratio of leg thickness in the direction of tapering. For example: A tapering factor 0.5 implies that, in the direction of taper the thickness of leg is reduced to half. Similarly, a tapering factor of 0.25 means a reduction in thickness by four times in the direction of taper.

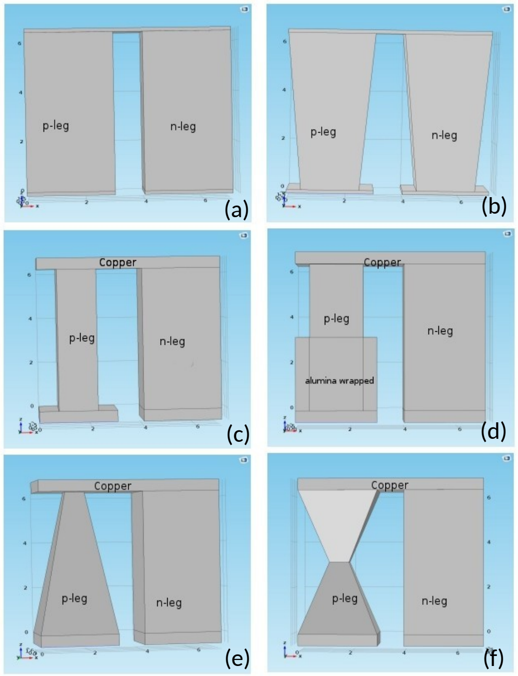

Figure 5. (a) Rectangular legs, (b) both legs tapered downwards with tapering factor 0.25, (c) p-leg reduced width by factor of 0.5, (d) p-leg half wrapped with alumina, (e) pyramidal shaped p-leg, (f) p-leg hourglass with tapering factor 0.25.

A trapezoidal leg with the lower end tapered with a factor of 0.25 (figure 5(b)). Asymmetric rectangular legs with one leg thinner than the other has been shown in figure 5(c). Thermal conduction on half wrapped (figure 5(d)) with alumina in p-leg is also included in the study. Pyramid shaped p-leg and hourglass geometry with half p-leg tapered in one direction and other half tapered in opposite such that both tapered end meet at center of leg length has been shown in figure 5 (e) and (f) respectively.

3. Results and Discussion

A theoretical analysis of thermoelectric unicouple is carried out on various geometries and shapes of thermoelectric legs including tapered p- or n-leg with different tapering factors, different thickness of p- or n-leg within a unicouple and hourglass shaped legs. In figure 6 the variation of terminal voltage for different shapes, specially in p-leg of the unicouple are shown. Terminal voltage has been calculated by taking the surface maximum of the p-leg lower end, from where current is injected. The plot shows that the electrical voltage increases as the tapering factor of p-leg altered. This is due to reducing the overall electrical resistance of the leg. The input current signifies the load attached externally to the device, so on decreasing current the load resistance increases and hence potential drops across the terminals. P-leg with hourglass structure measures the higher terminal voltage among all.

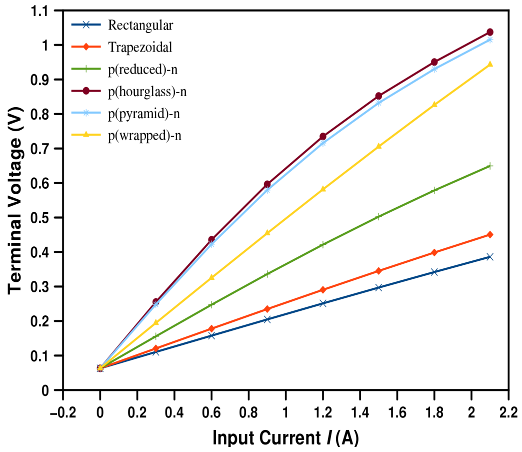

Figure 6. Terminal voltage of different shaped pn unicouple as a function of input current.

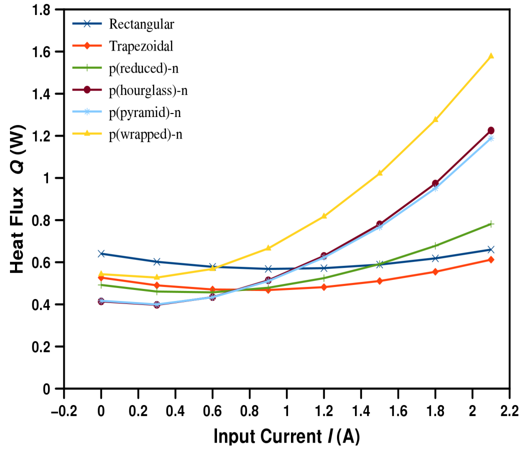

Figure 7. Conductive heat flux at cold end of different shaped pn unicouple as a function of input current.

From figure 7, it can be seen that the heat delivering capability of alumina wrapped p-leg increases as current increases, among all other shapes. Since thermoelectric device efficiency can be deduced either measuring electrical power or in terms of heat flow. Hence, it can help to enhance the thermoelectric efficiency at higher current as well.

Figure 8, demonstrates the simulation process for the various asymmetries induced unicouple thermoelectric. The surface profile is showing temperature variation while the the arrow in the volume shows the conductive heat flux in the *z*-direction.

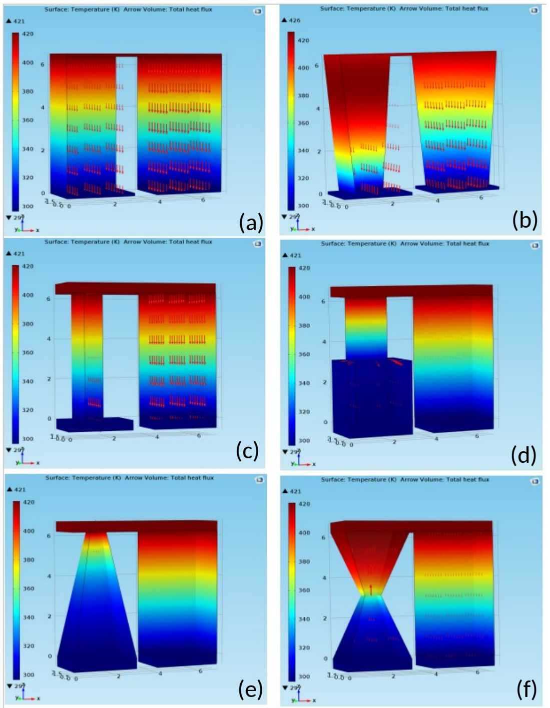

Figure 8. Surface temperature and conductive heat flux at an input current of 0.9 A.

Surface potential profile and volume current density are shown in figure 9. A constant current of 0.9 *A* has been allowed to flow through the device. Since the current is constant throughout the length of the p-leg, but crossectional area changes, this reflects in the electrical resistance expression and thus terminal voltage varies for different shape and size of the leg.

4. Summary

Simulation of different shapes of Mg_2Si based material has been carried out and single unicouple terminal voltage are measured. Temperature difference of 125*K* is maintained between the both ends. Using “COMSOL Multiphysics's Thermoelectric Effect” node, a finite element simulations have been performed on different shape and size of the thermoelectric legs, specially p-leg. The measured terminal voltage of a unicouple is observed to increase on introducing the various asymmetries in the leg geometry. It is observed that, the geometry with hourglass shaped p-leg and rectangular n-leg shows the higher voltage across the ends. The inclusion of asymmetry in p-legs can act as a potential way to enhance the efficiency of the thermoelectric unicouple. Furthermore, thermoelectric materials with different Seebeck coefficients and thermal conductivities can be explored in combination with various leg geometries.

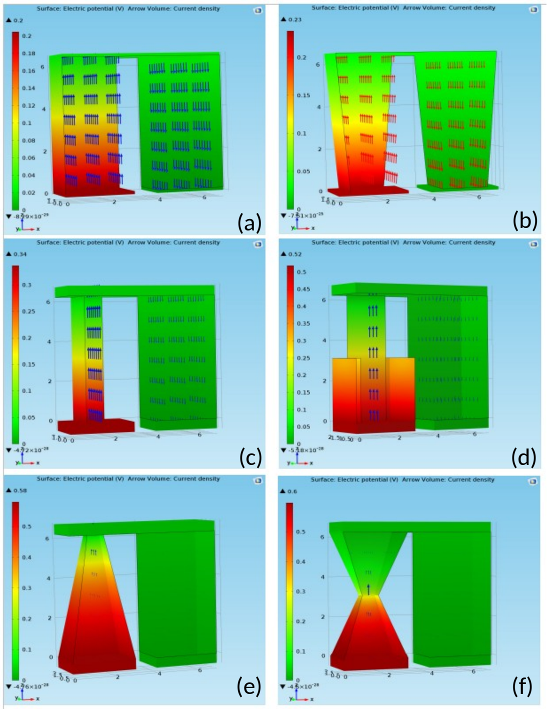

Figure 9. Electric potential and current density at an input current of 0.9 A.

5. Acknowledgments

This work was supported in part by IIT Bombay IRCC seed grant and partly by ARCI-Center for Automotive Energy and Materials, IIT Madras Research Park, Chennai.

6. References

1. H. Julian Goldsmid, *Introduction to Thermoelectricity*, 1-5, Springer Series in Materials Science (2009)

2. Ahmet Z. Sahin et al., The Thermoelectric as Thermoelectric Power Generator: Effect of Leg Geometry on the Efficiency and Power Generation, *Energy Conversion and Management*, 65 (2013) 26-32

3. Christophe Goupil et al., Thermodynamics of Thermoelectric Phenomena and Applications, *Entropy*, (2011), 13, 1481-1517

4. Yu Mu et al., Effect of Geometric Dimensions on Thermoelectric and Mechanical Performance for Mg_2Si-based Thermoelectric Unicouple, *Materials Science in Semiconductor Processing*, 17 (2014) 21-26

5. COMSOL Multiphysics 5.1, Heat Transfer Module User's Guide

6. H. Ihou-Mouko et. al., Thermoelectric Properties and Electronic Structure of p-type Mg_2Si and $Mg_2Si_{0.6}Ge_{0.4}$ Compounds Doped with Ga, *Journal of Alloys and Compounds*, 509 (2011) 6503–6508.

7. W. Liu et. al., Convergence of Conduction Bands as a Means of Enhancing Thermoelectric Performance of n-Type $Mg_2Si_{1-x}Sn_x$ Solid Solutions, *Physical Review Letters*, 108 (2012) 166601.