Thickness Designs for Micro-Thermoelectric Generators using Three Dimensional PDE Coefficient-Comsol Multiphysics 4.2a Analysis

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Abstract: This paper reports the optimal thickness and gap size for optimal output power between n-type and p-type silicon germanium (SiGe). The results showed that as thickness (tSiGe) decreased from 200 to 10 μm, the power output increased from 0.011 to 0.19 Watts and decreased to 0.0008 Watts across the diffusion barrier between (tCu/tSiGe). When copper thickness (tCu) increased from 10 to 150 μm, the power continued to decrease from 0.0008 to 0.00033 Watts. As the tCu in the gap (tgap) decreased from 150 to 10 μm, the power crossing the gap decreased from 0.0008 to zero Watts. The power crossing the tgap increased from zero to 0.0008 Watts when the tgap was decreased from 100 to 0.1 μm. These results showed that the optimal tCu and tSiGe on diffusion barrier should be 10 μm and the tgap should be 0.1 μm. The tCu along the tgap should be 150 μm.

Keywords: Micro-thermoelectric generator, Finite element analysis, Seebeck effect, Thermal conductivity, Electrical conductivity, tCu, tSiGe, p-type SiGe, n-type SiGe, tgap.

1. Introduction

Predicting the optimum thickness and gap size between n-type and p-type legs of micro thermoelectric devices are the major challenges in designing micro thermo electric generators. Recently, researchers have shown that the thickness of both electrode and thermoelectric layers can be estimated using 3-D Finite Element Methods [1-4]. However, determination of the optimum gap size remains a major challenge. To solve this problem, we have used the Partial Differential Equation (PDE) Coefficient form (c) in Comsol Multiphysics 4.2a to incorporate matrices of thermal conductivity (K), electrical conductivity (σ) and Seebeck coefficient (α) into 3D modeling. The thermoelectric materials evaluated with this approach are n-type and p-type SiGe [5, 6]. Comsol Multiphysics was then used to design micro thermoelectric generators and analyze voltage, current, and power, as a function of copper thickness (tCu), SiGe thickness (tSiGe), and gap size (tgap), as shown in Figure 1.

In this research we investigated three designs. In the first design, the width (w) and length (L) of both Cu and SiGe were fixed at 50 μm, the tgap was fixed at 100 μm, and the tSiGe was varied from 10 to 200 μm. In the second design, the tSiGe was fixed at 10 μm while the tCu varied from 10 to 200 μm, the tgap was fixed at 100 μm. In the third design, both tCu and tSiGe were fixed at 10 μm and the tgap was varied from 0.1 to 100 μm. The thermoelectric power was determined as it crosses tCu, w, and tgap. The temperature gradient applied was from 50 K to 500 K with ΔT=450 K.

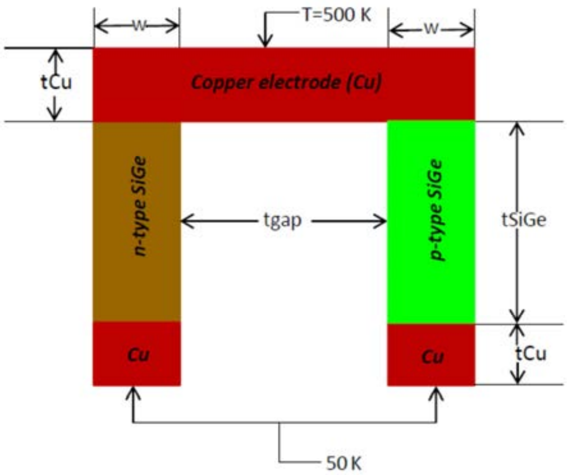

Figure 1. Schematic diagram showing the 1-dimension geometrical configuration of the designed micro thermoelectric generator.

2. Use of Comsol Multiphysics 4.2a: PDE Coefficient Form (c)

The PDE coefficient form is part of the Comsol Multiphysics computation tool, which allowed us to incorporate the thermoelectric materials' properties into matrix form which allows us to solve for voltage as a function of temperature. Assuming a steady state condition, the thermal conductivity (λ), electrical conductivity (σ) and Seebeck coefficient (α), were then substituted into thermoelectric equations (1) and (2) as

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described in [7], the variables 'T' and 'V' stands for temperature and voltage respectively. The gradient matrix in x, y, z directions is represented by Δ.

$$-\nabla((\sigma\alpha^2 T + \lambda\nabla T) - \nabla(\sigma\alpha T\nabla V) = \sigma((\nabla V)^2\alpha\nabla T\nabla V) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$\nabla(\sigma\alpha\nabla T) + \nabla(\sigma\nabla V) = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

In order to form matrices which will be used to analyze voltage as a function of temperature, equation (1) was assigned symbols 'c' and 'f' as seen in equation 3 and 4.

$$c = -\nabla((\sigma\alpha^2 T + \lambda\nabla T) - \nabla(\sigma\alpha T\nabla V) \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

$$f = \sigma((\nabla V)^2 + \alpha\nabla T\nabla V) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

'c' represents the diffusion term in PDE coefficient form shown in [8], while 'f' is the source term as shown in equation 5. Equation 5 represents the domain portion of thermoelectric materials and was used to input the parameters of thermoelectric layers into PDE coefficient form for both n-type and p-type SiGe. Equation 6 is the Newman domain boundary (upper boundary of the copper electrode). Equation 7 is the Dirichlet boundary and was used to assign temperatures on the hot side and cold side using PDE tool in Comsol Multiphysics. Using Dirichlet boundary the upper copper electrode was set at 500 K and the lower copper electrode was set at 50 K.

$$e_a\frac{\partial^2 u}{\partial t^2} + d_a\frac{du}{dt} + \nabla.(-c\nabla u - \alpha u + \gamma) + \beta.\nabla u + au = f;\ \ in\ \Omega \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

$$n.(c\nabla u + \alpha u - \gamma) + qu = g - h^T\mu;\quad on\ \partial\Omega \ldots\ldots\ldots(6)$$

$$u = r;\quad on\ \partial\Omega \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(7)$$

The symbol Ω represents domain or region in which PDE is used to solve problems. From equations 5 and 6, we can see that the symbol 'c' represents heat flow in a device by diffusion; other constants (e, d, γ, β, a) are not relevant to our research because they represent properties not related to our simulation design. The only terms used in our designs are the source term 'f' and diffusion coefficient termed as 'c'. Therefore, equation 5 reduces to $\nabla.(-c\nabla u) = f$, where μ represents the field variables matrix in PDE coefficient form, for solving temperature and voltage as seen in equation 8.

$$\mu = \begin{pmatrix} T \\ V \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (8)$$

Since the PDE coefficient form section in Comsol needs data in the form of special matrices, it was necessary to derive them using equation 3 and 4. Therefore, rearranging equations 3 and 4; we get the linear matrices shown in equations 9 and 10.

$$c = \begin{pmatrix} \lambda + \sigma\alpha^2 & \sigma\alpha T \\ \sigma\alpha & \sigma \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (9)$$

$$f = \begin{pmatrix} \sigma((\nabla V)^2 + \alpha\nabla T\nabla V) \\ 0 \end{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (10)$$

The thermal electric material constants α, σ, and λ, in equation 9 and 10 were then used to create a program in PDE Coefficient form section. This program was then used to compute temperature (T) versus voltage (V). Since the current density and the area ($A = 2.5 \times 10^{-9} m^2$) of thermoelectric device is known, equation (11) was then used to calculate current from J = I/A, where I is the current and J is the current density.

$$E = \alpha\nabla T - \rho J \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

The product of voltage (V) and current (I) in equation 12 gave power (P) crossing at any point on the 3-D pie (π) shape of thermoelectric device.

$$P = [\sigma_n(\alpha_n\nabla T - E) + \sigma_p(\alpha_p\nabla T - E)] * A * V \ldots\ldots(12)$$

Where σ_n is electrical conductivity of n-type SiGe, σ_p is the electrical conductivity of p-type SiGe, α_n is the Seebeck coefficient of n-type SiGe, α_p is the Seebeck coefficient of p-type SiGe and, E is the electric field along x, y, z directions.

3. Results and Discussion

The simulation results showing 3-D temperature distribution in micro thermoelectric generator is depicted in Figure 2. The hottest side is the red color showing the temperature distribution from 500 K at the top of a 10 μm thick layer of copper electrode, while the coldest side is the blue color (50 K) at the bottom of a 10 μm thick copper layer on both legs. The yellow color represents temperature distribution in thermoelectric layers between the two copper electrodes. The two thermal legs are connected at the top by a copper electrode (labeled as tgap in Figure 1) which indicates uniform temperature distribution of 500K.

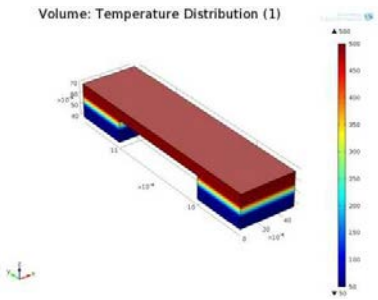

Figure 2. The 3-D temperature distributions in one of the designed micro thermoelectric generators with maximum gap size of 100 μm.

The results in Figure 3 (a) show that as the thickness of n-Type SiGe layer increased from 10 to 200 µm, the highest voltage generated was 0.078V because thermal gradient tends to increase as the thickness increases. On the other hand, In Figure 3(b), as the thickness of thermoelectric layer decreased from 200 to 10 µm, the current increased from 0.135A to 2.70A. Since current is inversely proportional to resistance, the thinner the thermoelectric layer the smaller the resistance and the higher the current. In addition, as the thermoelectric device gets thinner, there are less phonons generated as compared to a thicker thermoelectric device, the generated phonons reduce the current and power due to phonon/electron collisions, in turn, phonon/electrons collisions increased thermal resistance of the generator (K_g = t/2mλA), where 't' is the thickness, 'λ' is the thermal conductivity, 'm' is the couple of the thermoelectric legs and, 'A' is the area of the thermoelectric generator [9, 10].

In Figure 4 (a), as the thickness of p-type SiGe layer increased from 10 to 200 µm, the highest voltage generated was 0.078V, same as seen in n-type SiGe. Again these results proved that, as the device thickness is increased, the voltage increased due to accumulated thermal gradient. In Figure 4 (b), as the thickness of p-type thermoelectric layer decreased from 200 to 10 µm, the current increased from 0.131A to 2.51A. This current is 0.19A less than the 2.70A calculated for n-type SiGe because in n-type device there are more electrons as compared to p-type thermo electric leg which has fewer electrons and more holes.

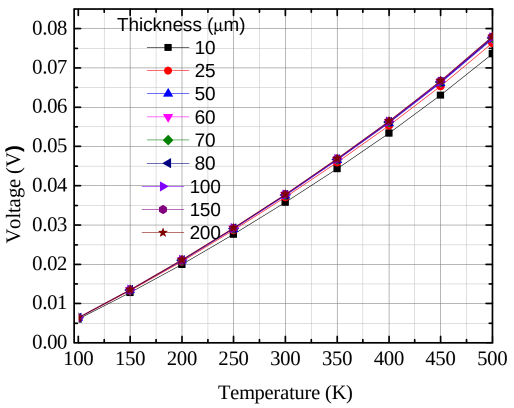

Figure 3 (a). The variation of voltage with temperature as the thickness of n-Type SiGe is varied from 10 to 200 µm.

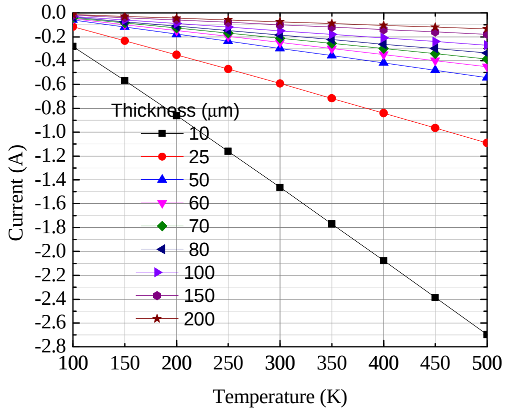

Figure **3 (b).** The variation of current with temperature as the thickness of n-Type SiGe is varied from 10 to 200 µm.

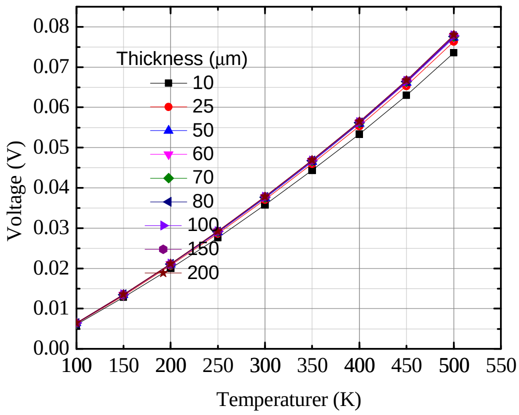

Figure 4 (a). The variation of voltage with temperature as the thickness of p-Type SiGe is varied from 10 to 200 µm.

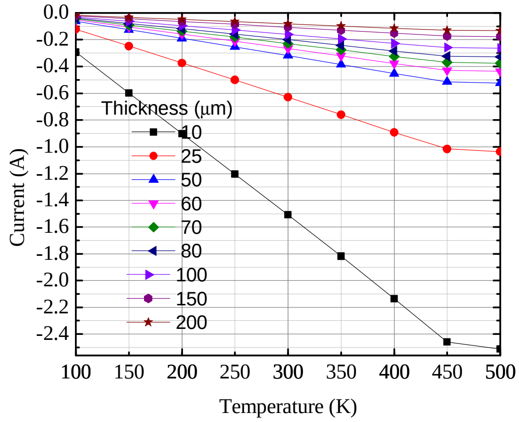

Figure 4 (b). The variation of current versus temperature as the thickness of p-Type SiGe is varied from 10 to 200 µm.

The voltage and current in Figure 3 and 4 were then used to calculate power across both n-type and p-type SiGe layers. The results shown in Figure 5 (a) indicate that as the thickness of n-type SiGe layer decreased from 200-10 µm, the power through the n-type SiGe increased from 0.011 to 0.199 Watts. This is consistent since the thermoelectric power is directly proportional to current which increases as the thermoelectric layers become thinner (Figures 3b and 4b). The power across p-Type SiGe (Figure 5 b) increased from 0.010 to 0.185 Watts as the p-type SiGe layer thickness decreased from 200-10 µm. This power is 0.014 Watts less than the 0.199 Watts generated in the 10 µm thick n-Type SiGe layer.

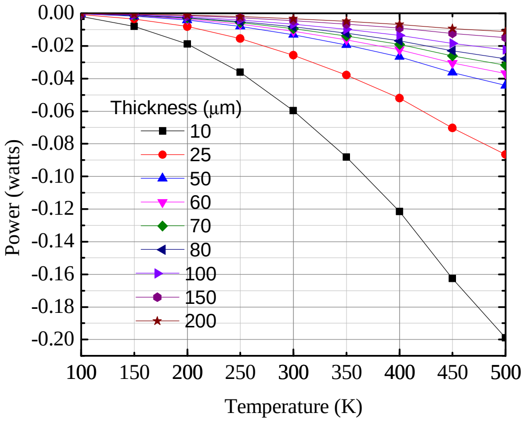

Figure 5 (a). The variation of power with temperature as the thickness of n-Type SiGe is varied from 10 to 200 µm.

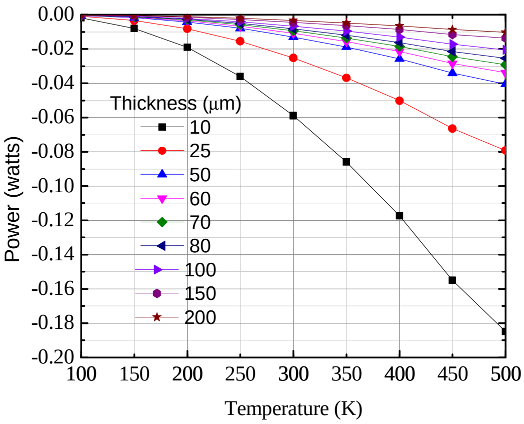

Figure 5 (b). The variation of power versus temperature as the thickness of p-Type SiGe is varied from 10 to 200 µm.

Figure 6 (a) shows the variation of power versus arc length of tCu. The results showed that as the thickness of the copper electrode decreased from 150 to 10 µm, the power passing from thermo legs to the copper electrode improved from 0.0003 to 0.0008 Watts. This means that the 0.19 Watts across the 10 µm of SiGe layers, decreased to 0.0008 Watts when analyzed across the diffusion barrier between tCu/tSiGe layers. In addition to that, when tCu along the tgap was decreased from 150 to 10 µm, the power crossing the tgap decreased from 0.0003 to zero W atts (Figure 6a and 6b). The power crossing the gap in Figure 6 (b) increased from zero to 0.0008 Watts when the tgap was decreased from 100 to 0.1 µm.

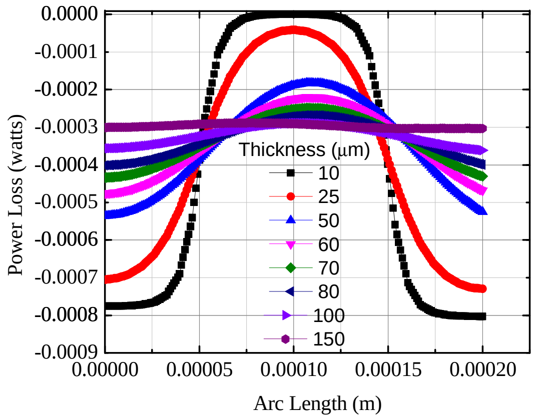

Figure 6 (a). The variation of power with arc length as the thickness of copper electrode is varied from 10 to 150 µm.

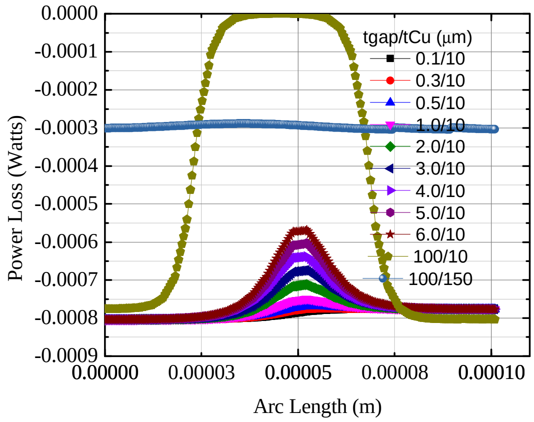

Figure 6 (b). The variation of power with arc length of tCu as the tgap of copper electrode is varied from 100 to 0.1 µm.

The final design layout of the micro thermoelectric generator showing the thickness of thermoelectric layer (tSiGe), the width (W), the length (L), the gap (tgap), and the thickness of copper electrode (tCu) is summarized in Table 1.

Table 1. Parameters of the designed micro thermoelectric generator.

Parameters	Value (µm)
W	50
L	50
tgap	0.1
tSiGe	10
tCu	10
tCu (tgap)	150

4. Conclusions

The results showed that as the thickness of SiGe layers decreased from 200-10 µm, the power analyzed across n-type SiGe increased from 0.011 to 0.199 Watts, and that from p-type SiGe increased from 0.010 to 0.185 Watts; because, thermoelectric power is directly proportional to the current which tends to increase as the thermoelectric thickness gets thinner. We noted that there is more power loss from thermo electric layers to electrode layers as the power crosses the diffusion barrier. The 0.19 and 0.185 Watts from both n-type and p-type thermo electric layers reduced to 0.0008 Watts after crossing the diffusion barrier. Also, as the thickness of copper electrode decreased from 150 to10 µm, the power induced from thermo legs to copper electrode improved from 0.0003 to 0.0008 Watts. This means that the 0.19 and 0.185 Watts analyzed across 10 µm of SiGe layers, increased to 0.0008 Watts when the tcu was reduced to 10 µm. In addition, when tCu along the gap was increased from 10 to 150 µm, the power crossing the gap increased from zero to 0.0003 Watts. This means that the electrode layer between the thermo legs should be thicker, approximately 150 µm. However, to maintain the maximum output power (0.0008 Watts) crossing the gap between n-type and p-type legs, the gap size should be 0.1 µm; but, depending on fabrication capability the gap size can be varied from 0.1to 6 µm, the power crossing the gap will degrade from 0.0008 to 0.00055 Watts respectively. We expect that, to obtain 1.0 Watt for the device fabricated using SiGe as thermoelectric layer (TE), we will need to fabricate 625 pairs of micro thermoelectric generators having both n-type and p-type, same as having 1250 thermo legs on a wafer.

5. References

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6. Acknowledgment

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