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Comparative analysis of thermoelectric behavior of molybdenum silicide ($MoSi_2$) and bismuth telluride (Bi_2Te_3)

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A comparative analysis of the thermoelectric behavior of Molybdenum Silicide and Bismuth Telluride using the COMSOL-Multiphysics platform is presented. Parameters like temperature distribution, potential distribution, figure of merit all the way through the length of the model and isothermal contours for these materials are reported. The outcomes of the modeling and simulation have revealed the potential use of Bismuth Telluride in thermoelectric applications at low temperature applications whereas Molybdenum Silicide is utilized as thermoelectric materials at high temperatures applications.

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1. Introduction

The quest for energy resources which reduces our reliance on fossil fuels is ever growing. This quest has led to vital regimes of exploration in direct conversion of thermal-electrical energy conversion via thermoelectricity. Thermoelectric materials are competent in openly and reversibly converting heat into electrical power. Such materials pose significant impact on power generation and cooling. Several materials are being explored by researchers for improved efficiency in power generation and novel Peltier cooling applications [1,2,3]. Several materials are being checked for his or her thermal properties together in bulk and nanoscale system. Materials like tellurides exhibit properties that are encouraging enough to be used as thermoelectric materials [1,2,3] but owing to their poisonous personality, materials such as silicides are gaining precedence.

In our work, we model and study the thermoelectric behaviour of Molybdenum Silicide and Bismuth Telluride using COMSOL Multiphysics®. COMSOL Multiphysics® works in an influential interactive environment want to model and solve all types of scientific and engineering problems. The software provides a commanding integrated desktop environment with a Model Builder that offers an entire overview of the model and access to all or any functionality [4]. We specifically use the thermoelectric module of COMSOL designed to find out the influence of heating as well as cooling in devices and processes [5]. The module is furnished by such simulation gears to find out the phenomenon of heat transfer, conduction and convection which are frequently in alliance with supplementary physics, such as structural mechanics, fluid dynamics and electro-magnetics. The overall workflow of the heat transport module is well documented in [5]. A number of the sooner studies [6,7,8] have discussed methods of such theoretical modeling.

We have chosen two different materials to understand their thermoelectric properties, namely, Bismuth Telluride (Bi_2Te_3), Molybdenum Silicide ($MoSi_2$). Section 2 describes the model geometry and materials properties used for simulation. In section 3, we discuss the experimental set up to perform the simulation. The results and analysis are reported in section 4.

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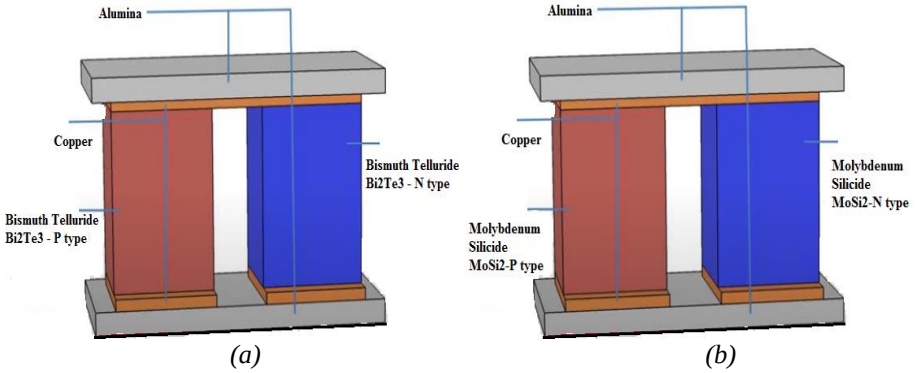
2. Modeling and Experimentations

2.1. Geometry

The thermoelectric material, both (Bi_2Te_3) and ($MoSi_2$) N-type and P-type are capped by two thin copper electrodes sandwiched by alumina plates are depicted in Figure 1(a) and Figure 1(b) respectively.



(a) *(b)*

Fig. 1. (a) Thermoelectric geometry of Bi2Te3; (b) Thermoelectric geometry of MoSi2.

The dimensions of the geometry are given in the table below.

Table 1. Geometrical parameters for TE module.

Design Parameters	**Value**
Alumina	3x1x.2 (mm)
Copper	1x1x0.1 (mm)
Bi2Te3	1x1x1.5 (mm)
MoSi2	1x1x1.5 (mm)
Pitch	0.5 (mm)
Voltage applied	0.1V- 0.5V

2.2. Material properties

Table 2 list the material properties of Bi_2Te_3 and MoSi2 which have been used as the input parameters of the simulation. These are given in the table below. Properties are chosen from the COMSOL Multiphysics material library. The input voltage range is kept from 0.1V to 0.5V. The standard value of the seebeck coefficient for copper is $6.5*10^{-6}$ V/K.

Table 2. Material properties of MoSi2 and Bi2Te3.

Property	**MoSi2**	**Bi2Te3**	**Unit**
Thermal Conductivity (k)	66.2	1.6	W/(m.K)
Density (ρ)	6240	7740	Kg/m^3
Heat capacity at constant pressure (C_p)	430	154.4	J/(kg.K)
Electrical Conductivity (σ)	3.28e6	1.1e5	S/m
Relative Permittivity (ε)	1	1	1
Seebeck Coefficient (S)	3.9e-6	2e-4	V/K

3. Experiment

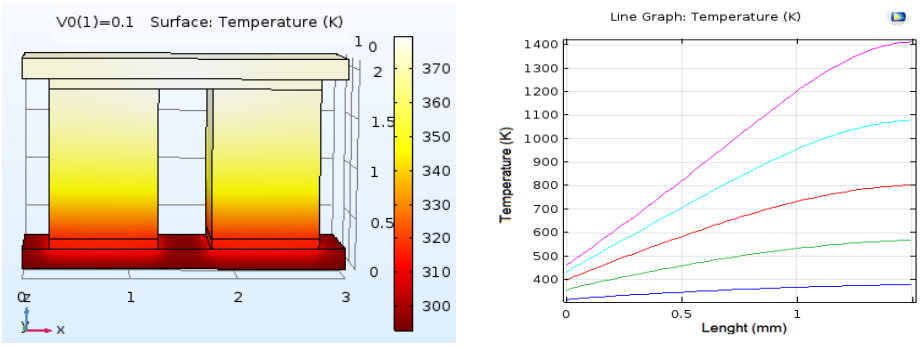
The bottom surface of alumina is held at temperature 273.5K. The copper electrode coupled to the lower leg of TE material (p-type) is connected to ground whereas copper electrode coupled to the lower leg of TE material (n-type) is provided the input voltage which in our case is from 0.1V – 0.5V. The top electrode and the lateral surfaces are thermally insulated. By applying the input potential, we are trying to build peltier effect with current going through the device and expecting cooling or heating at the top surface which is observed in the simulation.

4. Results and discussion

In this segment, we have presented the results which are figured from the simulation studies of the materials using the thermoelectric module of COMSOL. We look at different parameters which are temperature distribution all the way through the distance end to end of the module, potential distribution crossways the material, isothermal contours and the figure of merit across the span for both materials. The results are presented in the following figures (Fig.2 to Fig.6) and inferences therein are given at the end.

4.1. Temperature Distribution

Fig. 2(a) and 2(b) correspond to the surface temperature and variation in temperature all the way to the length of the TE material for Molybdenum Silicide (MoSi2). Variation in the temperature throughout the length of the module is figured from 273 K to 378 K for an applied voltage of 0.1V. The effect of heat rises the temperature to 378 K at other end producing a net temperature difference of about 105 K. Table 3 denotes the temperature at the top surface of the TE material for various input voltage values.



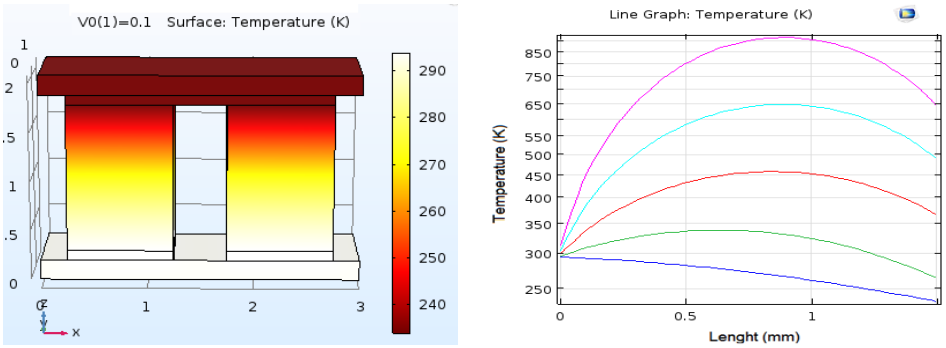
(a) *(b)*

Fig. 2. (a) Surface temperature for applied voltage; (b) Temperature variation across the length of MoSi2.

Table 3. Temperature variation on applied voltage.

Voltage	Temperature (MoSi2)	Temperature (Bi2Te3)
0.1V	378K	233K
0.2V	568K	264K
0.3V	802K	365K
0.4V	1074K	489K
0.5V	1400K	642K

Fig. 3(a) and 3(b) correspond to the surface temperature and variation in temperature all the way to the length of the TE material for Bismuth telluride Bi2Te3.



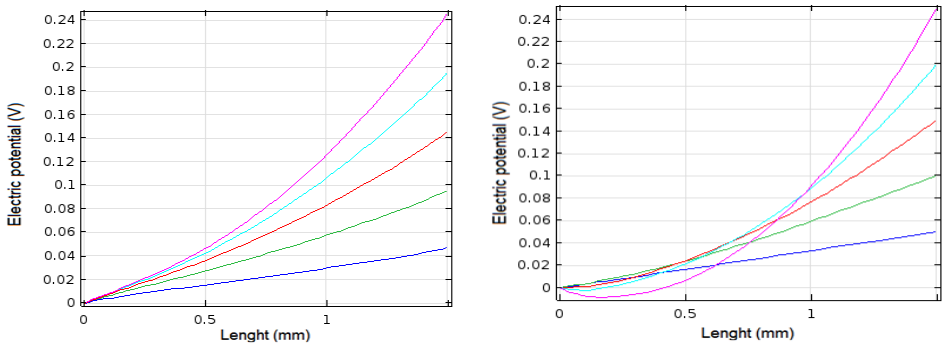
(a) *(b)*

Fig. 3. (a) Surface temperature for applied voltage; (b) Temperature variation across the length of Bi2Te3.

It is observed that $MoSi_2$ exhibits heating effect throughout the application of voltage whereas Bi2Te3 exhibits cooling effect at lower input voltages. The peak in temperature in Bi2Te3 is observed at the middle.

4.2 Electric potential Distribution

For a given material a certain potential difference needs to be maintained for driving a definite amount of current through the material. In the study, the simulation of heat transport in a material as a result of applied voltage allows us to examine the potential difference that would be obligatory to drive the desired current. Figures 4(a) and 4(b) illustrate these results.

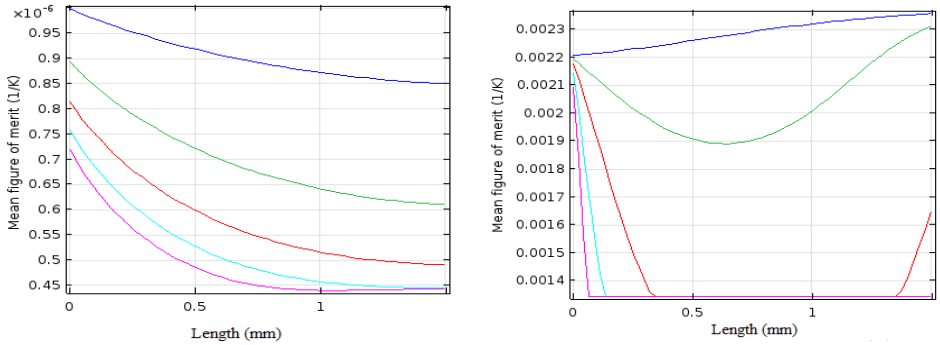


(a) *(b)*

Fig. 4. (a) Electric potential across the length of MoSi2; (b) Electric potential across the length of Bi2Te3.

4.3. Figure of Merit

The process of conversion of energy for power generation as well as cooling at a given point for maximum efficiency within the material is decided by the thermoelectric materials, figure of merit ZT. Figures 5(a) and 5(b) illustrate these results.

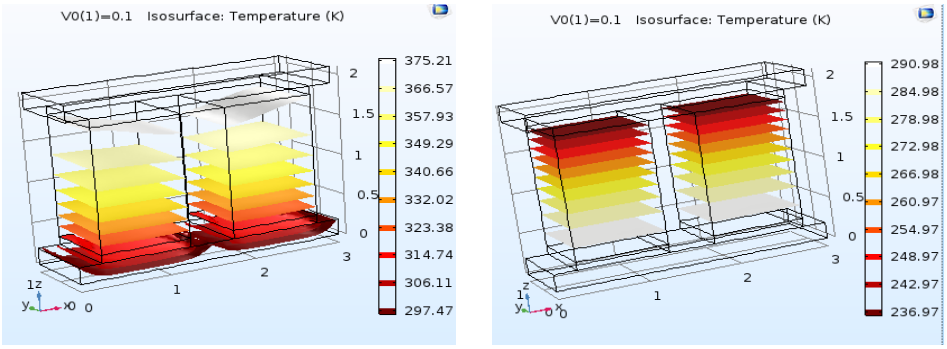


(a) *(b)*

Fig. 5(a). Figure of merit for MoSi2; (b) Figure of merit for Bi2Te3.

4.4. Isothermal Contours

These give the isosurfaces across the length of the material. The isothermal contours due to the temperature gradient set up by the flow of current for the material is shown in Figure 6(a) and (b).



(a) *(b)*

Fig. 6. (a) Isothermal Contours for MoSi2; (b) Isothermal Contours for Bi2Te3.

5. Inferences from the above model

It is observed that $MoSi_2$ exhibits heating effect throughout the application of voltage whereas Bi2Te3 exhibits cooling effect at lower input voltages. The peak in temperature in Bi2Te3 is observed at the middle. We infer that for Bi2Te3, the temperature at one end of the material reduces way below the room temperature as compared to the other end which is maintained at room temperature, causing Peltier cooling. It is concluded that the material can act as good thermoelectric materials. However, moreover, we also understand from the simulation that on appliance of upper voltages, past 0.2V, the temperature gradient decreases, limiting the Peltier Effect.

6. Conclusions

There are various explorations which are still being conceded out to comprehend the thermoelectric properties of pure and doped chalcogenides and skutterudites [9- 16]. In our work, COMSOL Multiphysics clearly demonstrates the model and displays the thermoelectric behavior of the materials taken. It has been observed that $MoSi_2$ exhibits heating effect throughout the application of voltage whereas Bi2Te3 exhibits cooling effect at lower input voltages. The highest

point in temperature in Bi2Te3 is noted at the middle. For Bi2Te3, the temperature at one end of the material reduces way below the room temperature as compared to the supplementary end which is kept at room temperature. However, in addition, we also understand from the simulation that on application of higher voltages, beyond 0.2V, there occur gradient in temperature which decreases.

]Further as a comparison, we observed that is a good thermoelectric material at low temperature. For high temperature applications $MoSi_2$ is a better alternative. Due to high- melting-point with excellent oxidation resistance, $MoSi_2$ is used in high-temperature furnaces because it can withstand prolonged exposure in air. Our study not only demonstrates the utility of the package for such applications but reflects the expected behavior of the selected materials apart from aiding in determining optimum parameters and doing a comparative analysis. No disbelief can be given that such computer simulations allow researchers and engineers to optimize parameters and improve process efficiency. It also helps in exploring materials and designs, thus reducing costs of manufacturing and production. The simulation is scalable and can be extended to study novel materials if the fundamental material parameters are known.

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