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Investigation on Thermoelectric Device Performance by Modeling and Simulations

Modelleme ve Simülasyonlar Yoluyla Termoelektrik Cihaz Performansının İncelenmesi

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ABSTRACT

This study investigates the performance of thermoelectric devices, specifically thermoelectric legs (TML), by using COMSOL Multiphysics simulations. Copper thermocouples having copper composite materials are investigated. The research uses finite element analysis to model heat and electric energy transfer within the thermoelectric system by considering whole surface temperature, electric potential difference, and iso-surface temperature. Simulation results indicate that the performance of TMLs in both *mm* and *nm* scales can be evaluated through the electric conductivity, thermal conductivity, and Seebeck values. The study explores impacts of composite material properties on thermoelectric device efficiency and highlights key challenges related to copper thermocouple integration and the complex behaviour of copper composite materials. This approach provides valuable insights for design of more efficient thermoelectric devices and addresses common issues encountered in experimental performance analysis

Keywords: COMSOL Multiphysics Simulation, Thermoelectric Device, Finite Element Analysis.

ÖZ

Bu çalışma, COMSOL Multifizik simülasyonlarını kullanarak termoelektrik cihazların, özellikle termoelektrik modül (TEM) performansını araştırmaktadır. Bakır kompozit malzemelere sahip bakır termokupllar incelenmiştir. Araştırma, tüm yüzey sıcaklığı, elektrik potansiyel farkı ve eş yüzey sıcaklığını dikkate alarak termoelektrik sistem içindeki ısı ve elektrik enerjisi transferini modellemek için sonlu eleman analizi kullanmaktadır. Simülasyon sonuçları hem mm hem de nm ölçeklerinde TEM'lerin performansının elektriksel iletkenlik, termal iletkenlik ve Seebeck değerleri aracılığıyla değerlendirilebileceğini göstermektedir. Çalışma, kompozit malzeme özelliklerinin termoelektrik cihaz verimliliği üzerindeki etkilerini araştırmakta ve bakır termokupl entegrasyonu ve bakır kompozit malzemelerin karmaşık davranışı ile ilgili temel zorlukları vurgulamaktadır. Bu yaklaşım, daha verimli termoelektrik cihazların tasarımı için değerli bilgiler sağlamakta ve deneysel performans analizinde karşılaşılan yaygın sorunları ele almaktadır.

Anahtar Kelimeler: COMSOL Multifizik Simülasyonu, Termoelektrik Cihaz, Sonlu Eleman Analizi

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Introduction

In device investigation, suitable electromagnetic energy is required to determine the thermal effect in a material. The required amount of energy for a material may be calculated by using the formula (Moorthy et al., 2017), (Sankar & Moorthy, 2025). The distribution of the energy while on modeling is mainly due to electromagnetic waves (Moorthy & Sankar, 2024). In that work, the spectrum of the waves is defined by wavelength ranges (Sankar, 2007). Those wavelength ranges are responsible for the energy transitions as well as temperature differences in the field of thermodynamic analysis (Özgür & Tosun, 2015), (Moorthy & Sankar, 2023). The force, field, and energy transformation may be difficult on experimental analysis (Sankar & Moorthy, 2025). So far, researchers are searching to optimize a suitable material for device fabrication (Udhaya Sankar et al., 2018). Yet, the suitable environmental circumstance is needed to analyse the device. Hence, researchers are approaching many modeling techniques like numerical thermal analysis, network modeling, and authentication approaches (Özakin et al., 2025; RajKumar et al., 2020; Sankar & Moorthy, 2020). In particular, thermal analysis, heat sinks, and temperature difference investigations in materials are required in modeling to examine the devices like thermoelectric device (Sankar et al., 2021; Yesildal & Yakut, 2017).

In the field of electronics, device fabrications are high-cost processes in the experimental research (Udhaya Sankar G et al., 2018; 2019). Yet, with the help of certain data collection related to material nature (Udhaya Sankar, 2022), a cost-effective simulation is possible (Udhaya Sankar et al., 2022). The thermoelectric legs (TML) attached in a thermocouple help to harvest energy based on materials chosen for TML. The major impact of thermocouples deals with chosen materials (Ganesamoorthy, 2023; Sankar et al., 2021). Copper-based composite materials are majorly used as thermoelectric materials for TML device performance analysis in recent advancements. Yet, the most common drawback in using copper thermocouple material for copper composite-based TML devices in experimental performance analysis is due to the same reference material. Therefore, this problem is investigated in the present work; finite element analysis is used for designing the thermoelectric device using COMSOL Multiphysics (Lara Ramos et al., 2019). This work studies the influence of copper-based thermocouples in the performance analysis of copper composite TML devices.

In simulation work, COMSOL Multiphysics with the theoretical background of finite element analysis and programming (Yushanov et al., 2011) is used. Energy transfer from one element to another element determines the whole heat transfer in the bulk $Cu_2Bi_2Te_3$ material (here, the element represents the e-numbered particles in the TML system). The various parameters in finite element analysis are referred to from the∇ matrix (Hu et al., 2015). The modeling and simulation part help to understand energy flow at the iso-surface model in *mm* and *nm*. Similarly, surface temperature and electric potential for the whole $Cu_2Bi_2Te_3$ bulk material are discussed by considering the whole material as an e-number of finite elements, which are represented in *mm* and *nm* scales. The results on thermal conductivity, Seebeck and electric potential for $Cu_2Bi_2Te_3$ material are discussed in the results and discussion section.

Materials and Methods

Method of Investigation

The structural, thermal, and electromagnetic computation solutions are found through the finite element analysis method with the boundary value problem in COMSOL Multiphysics (Pepper & Heinrich, 2017). On designing the TML device, a problem is faced at the high complexity in assembling the elements within the system. Here, the matrix function is used to determine ∇, which helps to resolve the element assembling problem while modeling.

Defining ∇ Function on Modeling

Fig.1a shows the modeling of thermoelectric leg in the rectangular system (in *mm*); Similarly, Fig.1b represents the formation of the rectangular system along with copper thermocouple material; it transfers heat energy source from bottom to top with respect to the system of coordinates(x, y, z). Energy transfer in the bulk composite $Cu_2Bi_2Te_3$ material is also considered as (x', y', z')in three dimensional TML systems. The material $Cu_2Bi_2Te_3$ having e-numbered finite elements (which can be expressed in *mm* as well as *nm* scales) that are arranged in pattern of 3 domains, 16 boundaries, 28 edges and 16 vertices are shown in Fig.1d. The heat and electric energy can be transferred from one element to another element in the TML device. Thus, the energy transfer can be investigated through coordinates and elements of system.

From Fig. 1c, the mesh generation in TML is for the element analysis, which states the matrix arrangement of elements in a rectangular three-dimensional system.

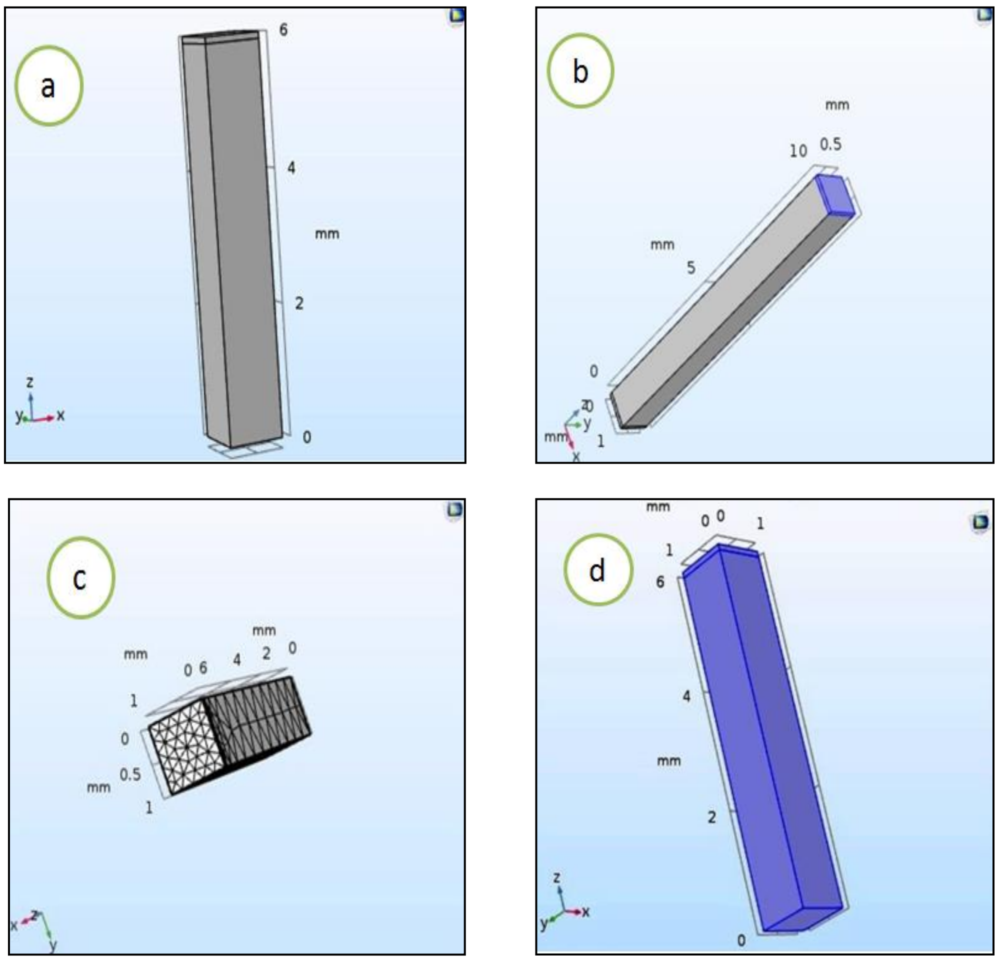
The heat/electrical energy source transfer is given in Equation 1.

$$\nabla = \sum_{i,j} \left| \boldsymbol{e}_{i,j} \right| \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} \qquad (1)$$

Modeling and Simulation

The model of TML device is constructed by using ∇ function through finite element analysis methodology (Hu et al., 2015). The parameters for the $Cu_2Bi_2Te_3$ bulk material are fed in the model builder tab on COMSOL Multiphysics (Ashby, 1997; Ganesamoorthy, 2023; Sankar et al., 2021). After that, Geometry for the TML is constructed; it may be varied from *mm* range as well as *nm* range. The mesh generation in the model is considering as$e$-numbered finite elements. In Fig.2a, the electric potential for the TML is modeled between the ranges of 0V to 50 x 10^{-3} V. The inside energy transformation between the thermocouple and TML is represented in the three-dimensional model as the *nm* range. Fig. 2b shows *nm* range of inner elements (layer by layer) modeled as an iso-surface temperature model. Here, the temperature range varied from 3.04°C to 57.87°C. Similarly, the whole surface temperature is modeled in *nm* range as shown in Fig.2c. Here, the temperature range varies from 0°C to 60°C. Fig.2d shows the TML model consisting of copper thermocouples and $Cu_2Bi_2Te_3$ bulk materials arranged as *e*-numbered finite elements in *nm* range at three-dimensional model.

Figure 1.
a) TML in mm, b) Thermocouples and the TML (mm), c) Element mesh generation in TML (mm), d) Arrangement of material $Cu_2Bi_2Te_3$ in TML (mm) and Copper thermocouple (mm).

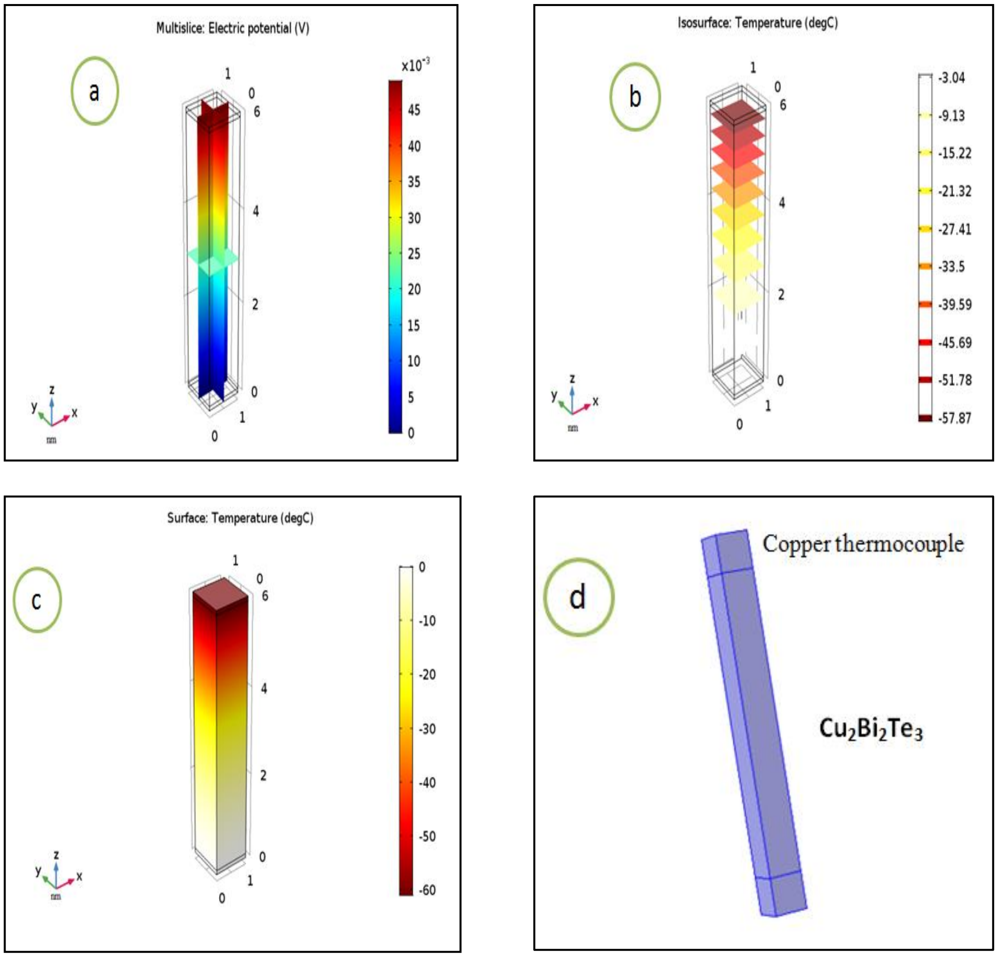


In simulation, the electric potential inside surface elements is analysed through a model as shown in Fig. 3a. The *nm* range of finite elements is analysed, and data are gathered from simulations. Similarly, Fig. 3b shows the electric potential model at the range of *mm*. Here, the data are collected in the *s.mm*$^{-1}$ and *ms.nm*$^{-1}$ scale range. Required data sets are given in the supplementary document. Fig. 3c is the thermoelectric device to analyse the performance of $Cu_2Bi_2Te_3$ TML.

The iso-surface temperature has been analysed for the TML of $Cu_2Bi_2Te_3$ material. The flow of heat flux towards the inward is shown in Fig. 4b. Here, *mm* range of TML has a temperature range in between 3.04°C and 57.87°C. Similarly, Fig. 4c shows that the *nm* range of TML has a temperature range in between 3.04°C and 57.87°C. Both models were analyzed at the same temperature range with different sizes, and the data were collected as thermal conductivity. Fig. 4a shows the TML of iso-surface temperature with the temperature range set between 294.65 K and 351.65 K.

Figure 2.

a) Electric potential of TML in nm, b) iso-surface temperature of TML in nm, c) surface temperature of TML in nm, d) Modeled TML in nm



The whole surface temperature is analysed in the TML model as shown in Fig. 5a at the range from 0°C to 60°C. Here, the Seebeck data had been collected as mV°C^{-1} for *mm* range scale and µV°C^{-1} for *the nm* range scale. Fig. 5b and Fig. 5c show the whole surface temperature TML model at the range of *mm* and *nm*, respectively. Here, the $Cu_2Bi_2Te_3$ TML is analyzed with respect to the temperature range from 0°C to 60°C.

Results and Discussion

The data are collected from three specific simulation models: electric potential instead of electric conductivity; iso-surface temperature instead of thermal conductivity; and whole surface temperature instead of Seebeck values. The entire TML model is analyzed in the range of *nm* as well as *mm* for the composite material ($Cu_2Bi_2Te_3$). During the electric potential simulation, the conductivity of the composite material $Cu_2Bi_2Te_3$ with respect to the copper thermocouple is gradually seen from electric potential (*smm^{-1}*) and electric potential (*snm^{-1}*) as shown in Fig. 6a and Fig. 6b, respectively. In the range of *mm*, the temperature is varied from 10°C to 60°C; while on simulation, the result of conductivity is gradually increasing from 70 σ to 140 σ. At 70°C, the peak of electric conductivity at 190 σ is due to the barrier potential of the composite material $Cu_2Bi_2Te_3$. Similarly, in the range of *nm*, the simulation result shows a U-shaped oscillation between the temperature range of 10°C to 30°C. After that, it gradually increases up to 50°C, as 170 σ. Again, it goes high at the temperature range of 60°C, as 185 σ. Then, it comes down as 165 σ when the temperature is raised to 70°C. It is due to the barrier potential breaking down in the composite material of $Cu_2Bi_2Te_3$.

Figure 3.

a) Electric potential of TML in nm, b) Electric potential of TML in mm, c) $Cu_2Bi_2Te_3$ TML Electric Potential

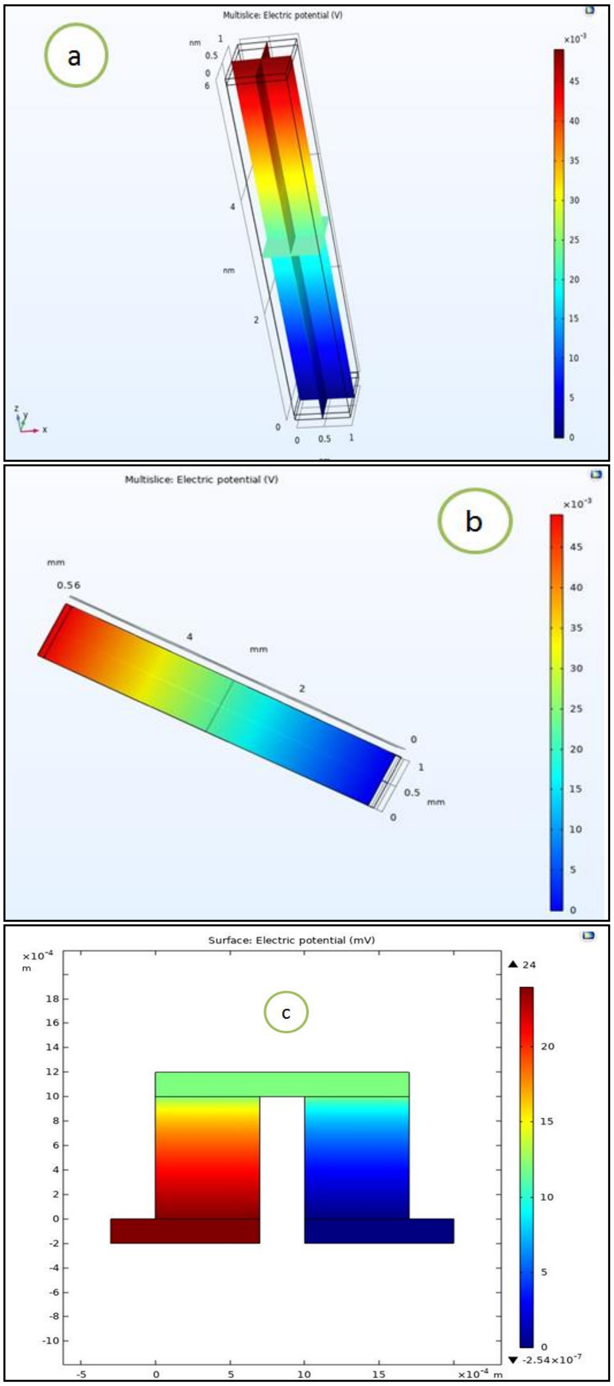


Figure 4.

a) $Cu_2Bi_2Te_3$ TMLiso-surface temperature (K), b) iso-surface temperature (°C) of TML in mm, c) iso-surface temperature (°C) of TML in nm

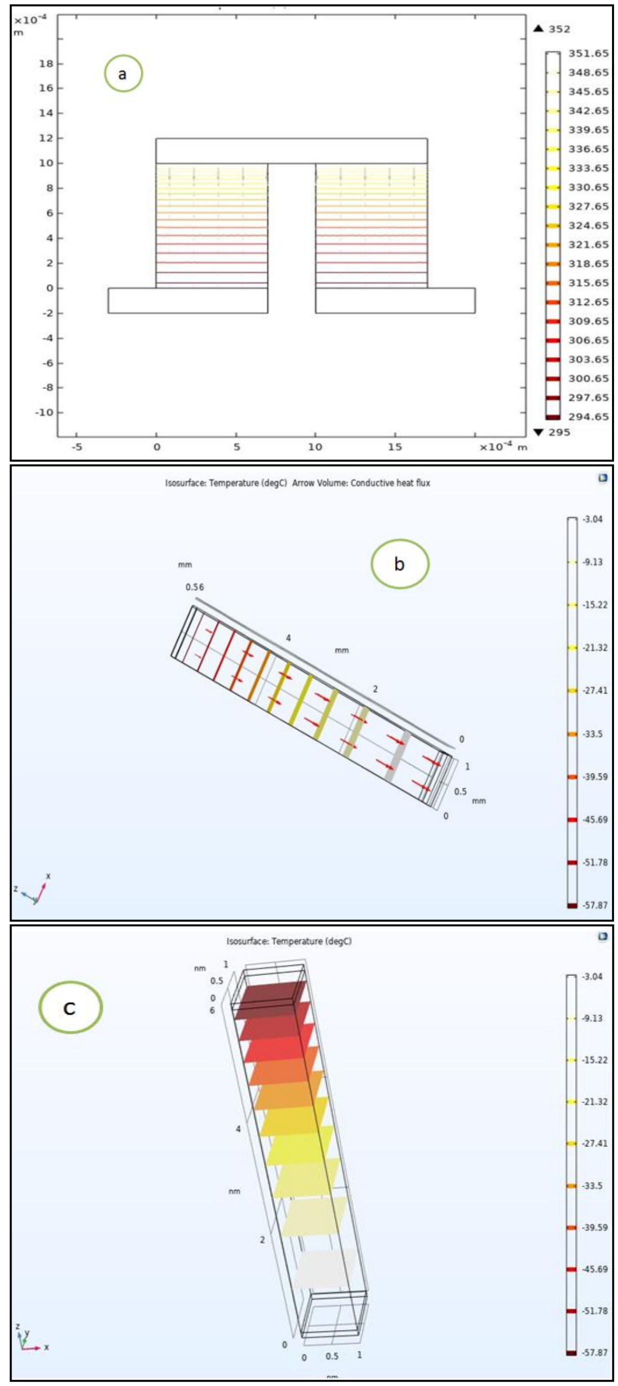
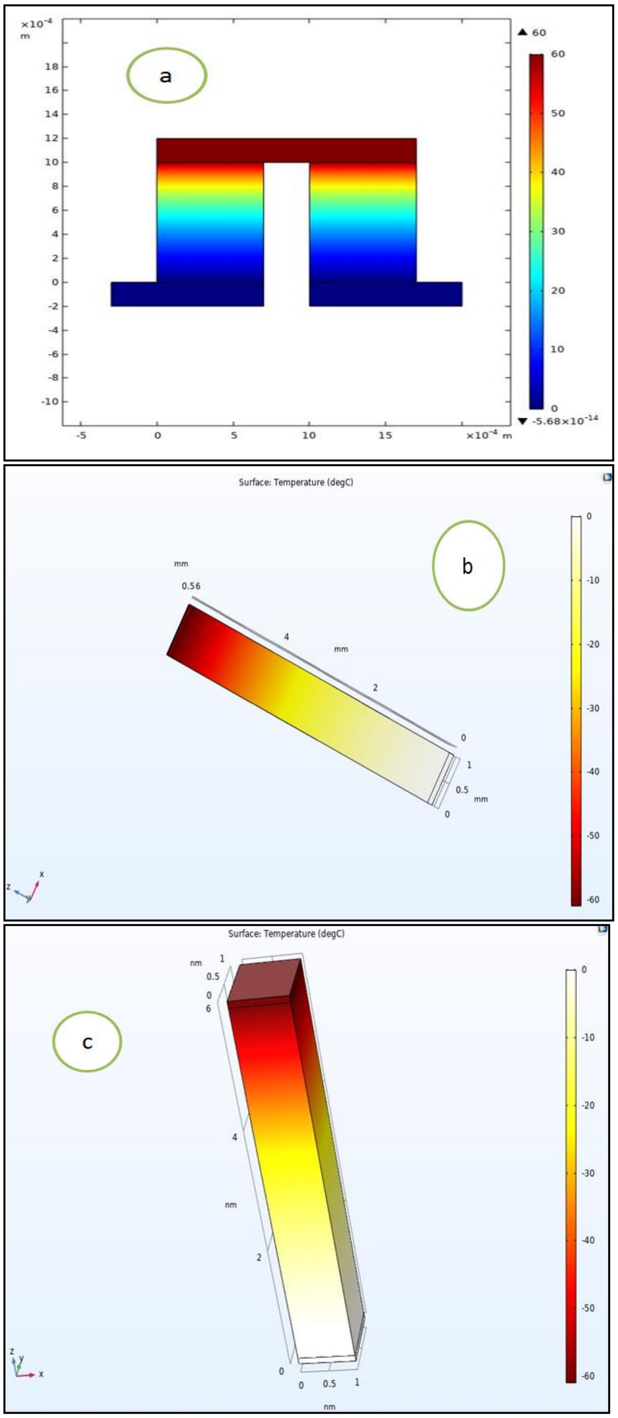
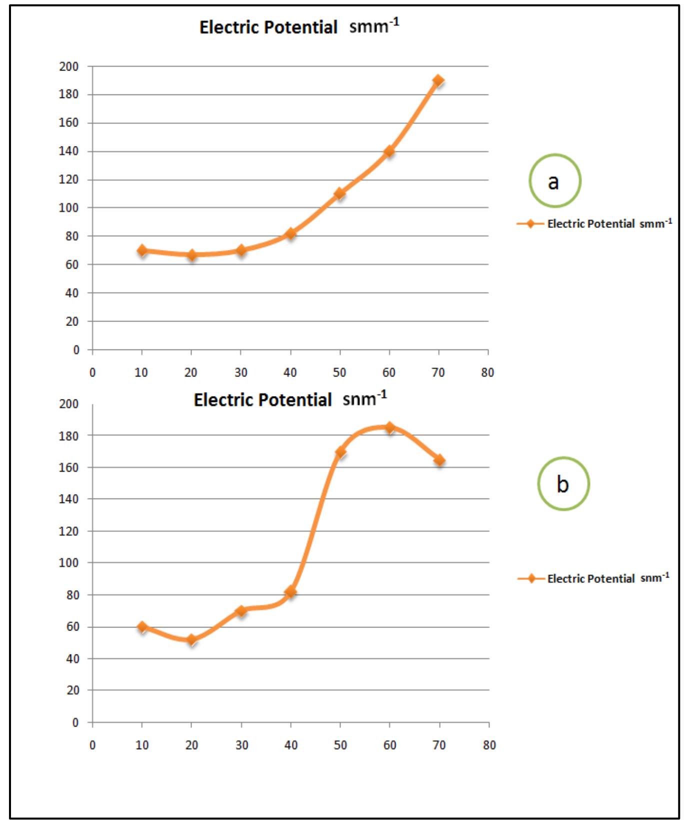


Figure 5.
a)$Cu_2Bi_2Te_3$ TML of whole surface temperature (°C), b) whole surface temperature (°C) of TML in mm, c) whole surface temperature (°C) of TML in nm



At the TML of $Cu_2Bi_2Te_3$, the iso-surface temperature of heat flux flows inside throughout the TML device. The moment of the elements in the TML acquired some vibration due to the temperature variation from the copper thermocouple (Southard & Andrews, 1929; Quiggle et al., 1937; Webster, 2021). In the range of *mm*, the thermal conductivity (k) values seem like a wave-like formation with

Figure 6.
a) Electric conductivity of TML - $Cu_2Bi_2Te_3$ in mm, b) Electric conductivity of TML - $Cu_2Bi_2Te_3$ in nm



respect to the temperature variation between 10°C and 70°C in the simulation. Most of the elements in the $Cu_2Bi_2Te_3$ TML are conductive as wave-like formations at 1.5 (k) and 2 (k) as shown in Fig. 7a, and these wave-like formations deal with the composite material vibration properties (Ganesamoorthy U. S., 2023). Similarly, the *nm* range of thermal conductivity deals with similar wave-like formations between the temperature ranges from 10°C to 70°C in simulation. Yet, the wave-like data set gradually decreases with respect to increased temperature as shown in the Fig.7b. and this may be due to the tightly packed elements in the $Cu_2Bi_2Te_3$ TML at the *nm* range. The maximum thermal conductivity of the $Cu_2Bi_2Te_3$ TML is acquired at 50°C and 70°C *mm* range and *nm* range, respectively

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Figure 7.
a) Thermal conductivity of TML - $Cu_2Bi_2Te_3$ in mm, b) Thermal conductivity of TML - $Cu_2Bi_2Te_3$ in nm

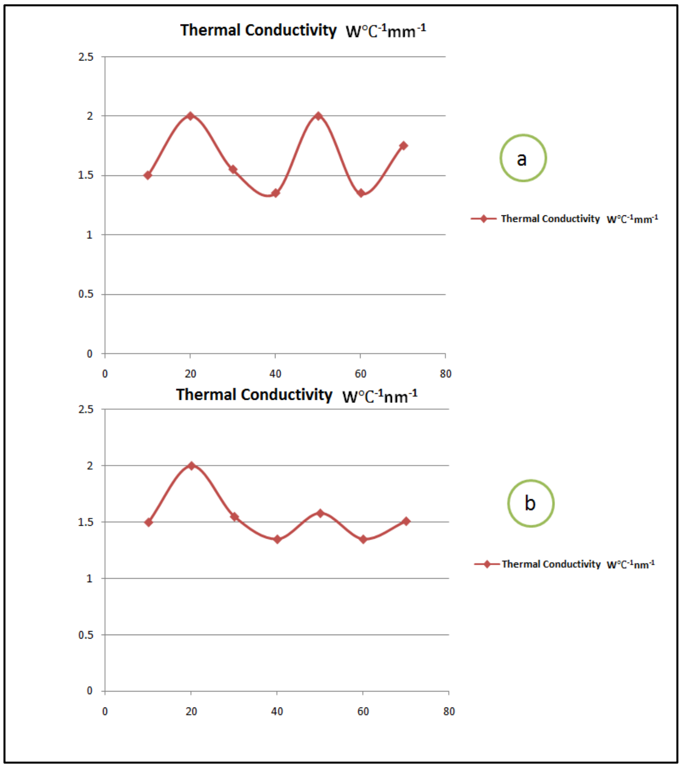
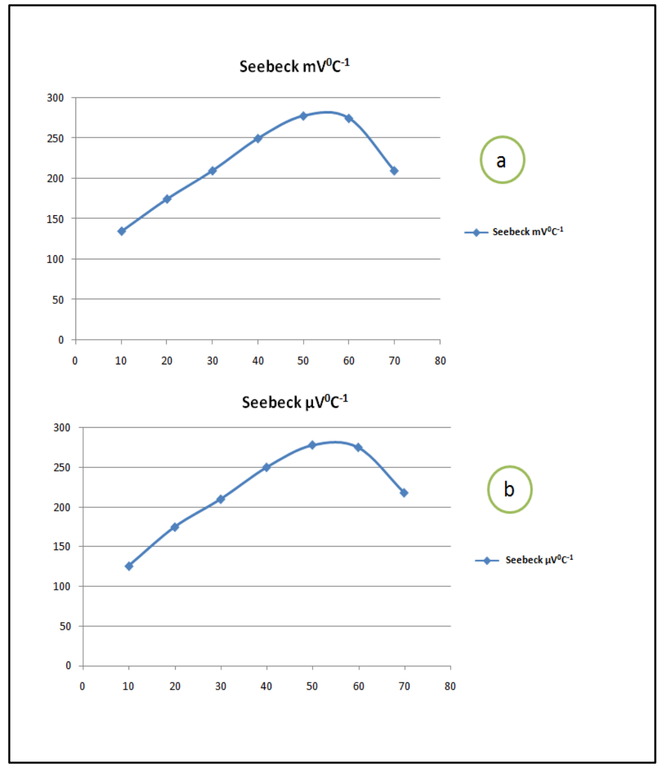


Figure 8.
a) Seebeck of TML - $Cu_2Bi_2Te_3$ in mm, b) Seebeck of TML - $Cu_2Bi_2Te_3$ in nm



In the modeling, the whole surface temperature of TML for the composite material of $Cu_2Bi_2Te_3$ (*mm* &*nm* range) is simulated between 10°C and 60°C, and these temperatures and Seebeck data collections in the system are shown in Fig. 5a. The resultant data were analyzed in mV and µV with respect to temperature as shown in Fig. 8a and Fig. 8b, respectively. Fig. 8a represents the Seebeck value increasing gradually with respect to the temperature and decreasing at a particular point. The maximum value of Seebeck at the growth point is due to coefficient phenomena at the TML (Lubikowski et al., 2015). The *mm* range TML generates 278 mV at 50°C. Similarly, the maximum Seebeck value is generated at 50°C in *nm* range as 278 µV. Thus, TML of composite material ($Cu_2Bi_2Te_3$) generates the coefficient value at 50°C as 278 S. The other necessary data are given in the supplementary document.

Conclusion

The COMSOL Multiphysics simulations conducted in this study reveal crucial insights into the thermoelectric performance of composite material ($Cu_2Bi_2Te_3$)-based TML devices. By examining composite material behaviour at both the *mm and nm* scales, the study identifies significant trends in electric conductivity, thermal conductivity, and Seebeck coefficients under varying temperature conditions. Notably, the results demonstrate that the inclusion of copper-based thermocouples can influence the energy transfer processes, with varying degrees of efficiency across different scales. The findings also emphasize the complex interaction between composite material properties and device performance, particularly the role of the $Cu_2Bi_2Te_3$ composite material in optimizing thermoelectric behaviour. Overall, this work underscores the importance of modeling and simulation-based approaches for addressing the challenges of designing and optimizing thermoelectric devices, which offers a cost-effective alternative to experimental methods and paves a way for further advancements in thermoelectric technology.

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G. Udhaya Sankar: Conception, Modeling, Simulation, Data Collection and Interpretation

C. Ganesa Moorthy: Analysis, Writing and Supervision.

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