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Optimization of Materials for Thermoelectric Leg Model Device

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ABSTRACT

A thermoelectric leg (TML) model is formulated by using finite element analysis (FEA) implemented in COMSOL Multiphysics. In the modelling approach, segmented thermoelectric legs demonstrate higher efficiency compared to non-segmented configurations. The simulations were performed for TML devices fabricated from Cu_2Te, $Cu_2BiSbTe$, and $Cu_2Bi_2Te_3$ materials. Prototype of TML geometry with dimensions of 1 mm × 1 mm × 2 mm (width × depth × height) was employed. The finite element analysis study investigates the influence of temperature, thermoelectric leg height, inlet temperature, and material selection on device performance. At 450 K, $Cu_2Bi_2Te_3$ generates an electric potential approximately 24% higher than that of $Cu_2BiSbTe$. Furthermore, at 615 K, the calculated electric potential is nearly 20% higher than values obtained using physical constants measured at different temperatures. The simulation results yield a Seebeck coefficient of 141 μV/K for $Cu_2Bi_2Te_3$, indicating its superior thermoelectric performance among the investigated materials.

Keywords: Thermoelectric leg, copper composite thermoelectric device, electronic material science.

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1. INTRODUCTION

Thermoelectric legs (TMLs) are devices that generate electrical energy from heat based on thermoelectric properties of the materials used. The performance of a thermoelectric device strongly depends on the selection of thermocouple and thermoelectric materials. In recent years, thermoelectric generators have received considerable attention as clean and sustainable energy solutions in response to increasing global energy demand, climate change concerns, and the need for environmentally friendly technologies [1, 2, 20, 22, 28, 29]. The performance of a TML device can be enhanced by modifying thermocouple materials while employing a single leg material, either n-type or p-type semiconductor. Various thermocouple materials are commercially available, including nickel, nickel–chromium alloys, nickel–aluminum alloys, iron, copper, Nicrosil alloys, molybdenum, and tungsten [9, 21, 30]. Among these materials, copper-based thermocouples are widely studied for thermoelectric performance analysis. Although copper thermocouples typically exhibit low efficiency, advances in technology have demonstrated that their performance can be significantly improved. Consequently, recent research efforts focus on enhancing thermo power and electrical conductivity while reducing thermal conductivity.

The present study investigates a thermoelectric leg model incorporating heat sinks and cooling mechanisms. The electric potential generated via the Seebeck effect is computed for different materials subjected to a temperature gradient between the hot and cold surfaces. This work compares thermoelectric performance of various copper based materials through finite element simulations using COMSOL Multiphysics.

The efficiency of thermoelectric devices is largely governed by material properties. Although copper is mosteffective in efficiency and widely used, copper based TML devices may exhibit performance limitations in thermoelectric legs [14]. To optimize this issue, the present work employs finite element analysis to simulate and evaluate the thermoelectric performance of Cu_2Te, $Cu_2BiSbTe$, and $Cu_2Bi_2Te_3$ materials. The influence of copper composite selection on the Seebeck coefficient, electrical potential, and thermal conductivity is analyzed. The modelling and simulations are conducted by using COMSOL Multiphysics with a strong theoretical foundation in finite element analysis [3, 5, 19]. Material properties were compiled from literature sources [22, 24, 26, 27], and heat transfer within the materials was optimized at the elemental level. The investigation framework is based on gradient (∇) operators [14], and the simulation results are discussed in detail. Future research directions are also outlined.

2. OPTIMIZATION

Finite element analysis (FEA) enables structural, thermal, and electromagnetic computations by solving boundary value problems consisting of equations [2, 5]. For thermoelectric leg applications, thermal behaviour and electrical potential can be accurately evaluated by using this method [11–14]. Device complexity is managed by representing systems through matrix equations derived from gradient (∇) operators. The thermoelectric leg geometry is designed in COMSOL Multiphysics, where shape and size are defined by using built-in geometry tools [5–9]. Material properties such as electrical conductivity, thermal conductivity, and Seebeck coefficient are selected from the material library [1, 14]. Thermoelectric device interfaces are applied to define boundary conditions, including hot-side and cold-side temperatures. Meshing is performed in using finite element analysis and numerical analysis, and it is carried out for various n-type TML configurations to evaluate temperature and voltage distributions [2, 5].

COMSOL supports three-dimensional modelling and allows time-dependent studies and stationary studies. It integrates multiple physics interfaces, such as electric potential, heat transfer in chosen material model, so that it is well suited for thermoelectric simulations. Governing equations can be directly implemented, and additional physics modules can be incorporated as needed [4, 8, 16]. The finite element method ensures high computational accuracy and computational efficiency.

2.1. Defined ∇ Function

A rectangular coordinate system is assumed for modelling the thermoelectric leg, as illustrated in Figure 1. Heat transfer occurs from the bottom to the top surface along the (x, y, z) coordinates, while the transformed coordinate system is represented by (x′, y′, z′). The finite element mesh consists of multiple elements distributed across three domains, sixteen boundaries, twenty-eight edges, and sixteen vertices, as shown in the iso-surface representation of the TML (Figure 2).

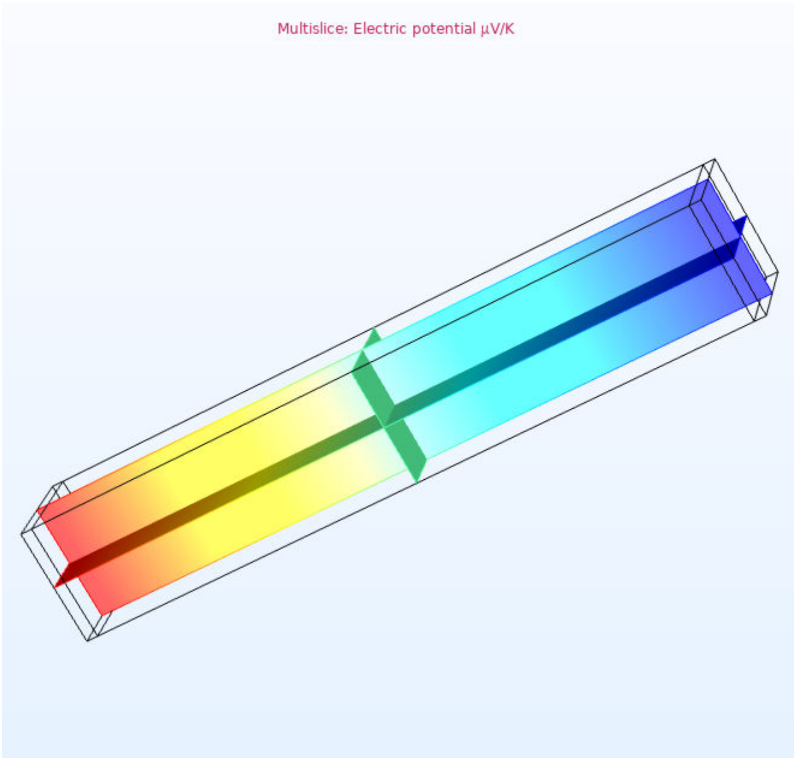

Figure 1. Electric potential of thermoelectric leg model.

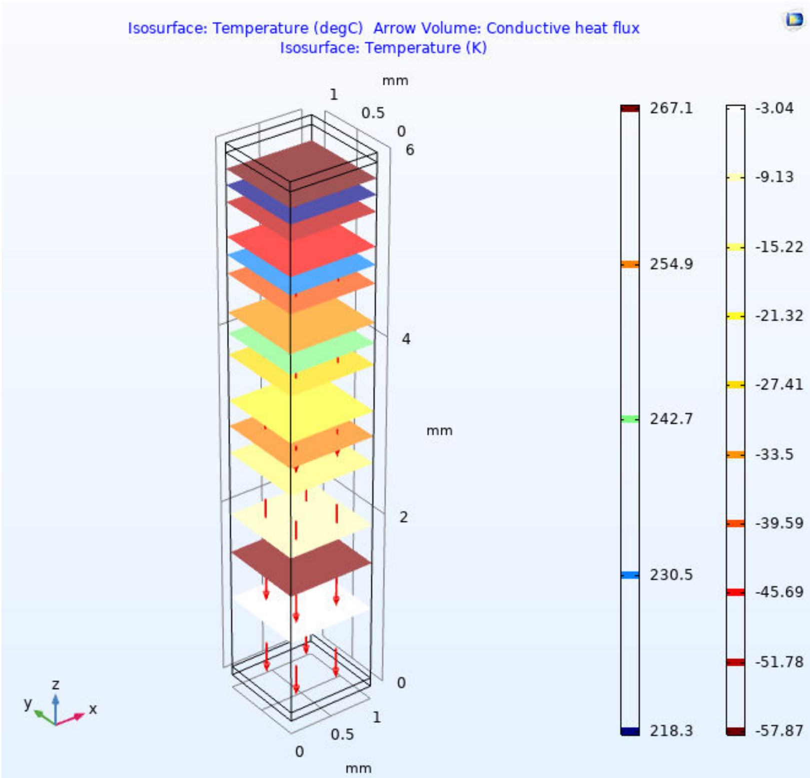

Figure 2. Iso-surface thermoelectric leg model.

Energy transfer between elements is analyzed through coordinate transformation and matrix representation. The element arrangement follows a 3 × 3 mesh structure, where heat and electrical energy propagation are described by using gradient operators and matrix transposition. To avoid negative numerical artifacts during simulation, the absolute values of element contributions are used. Consequently, the gradient operator (∇) represents the cumulative energy transfer across the transformed coordinate system [14].

2.2. Literature Background

Thermoelectricity was first discovered by Thomas Johann Seebeck in 1821, who observed that a temperature difference between two dissimilar materials produced an electric current [12]. This phenomenon, known as the Seebeck effect, forms the basis of thermocouples. The Peltier effect, discovered by Jean Charles Athanase Peltier, describes heat absorption or release at a junction when an electric current is applied [13]. Lord Kelvin later provided a thermodynamic explanation of these effects and predicted the Thomson effect [17,18].

The figure of merit (ZT), introduced in the mid-20th century, quantifies thermoelectric performance, while the thermoelectric quality factor characterizes semiconductor efficiency [10]. Thermoelectric devices are widely used in temperature sensing, solid-state cooling, and waste-heat energy conversion [17, 19, 26 – 30]. The Seebeck coefficient depends on temperature and crystal structure, when semiconductors offer higher tunability than metals [5, 10, 23]. All governing equations for Seebeck, Peltier, and Thomson effects are implemented in COMSOL Multiphysics for finite element analysis modelling.

2.3. Materials

The development of composite materials in the early 1990s renewed interest in thermoelectric research. Finite element analysis enables simulation of energy transfer processes such as thermal, electrical, and magnetic transport [6, 7, 14, 15]. In this work, COMSOL Multiphysics is employed to simulate electric potential and thermal energy transfer in Cu_2Te, $Cu_2BiSbTe$, and $Cu_2Bi_2Te_3$ materials.

2.4. Investigation method procedure

Thermoelectric legs consist of rectangular semiconductor blocks connected electrically in series or parallel and mechanically supported by insulating plates. Device efficiency depends on materials optimization by means of the temperature difference across the legs. Segmented thermoelectric legs, formed by stacking materials optimized for different temperature ranges, can enhance efficiency, although interface resistance may reduce electrical conductivity [5].

The simulation procedure includes:

a) Creating a stationary 3D COMSOL model for thermoelectric leg, including a thermocouple. A TML geometry of 1 mm × 1 mm × 2 mm is created by using the COMSOL Model Wizard.

b) Compiling thermoelectric material properties from literature and estimating missing data by using the Kopp–Neumann rule.

c) Running simulations for copper based composite (Cu_2Te, $Cu_2BiSbTe$, and $Cu_2Bi_2Te_3$) materials.

3. OPTIMIZATION RESULTS

In this optimization, Figure 3, 4 and 5 represent the performance of thermoelectric leg (TML) materials by using finite element simulations in COMSOL Multiphysics to determine optimal thermoelectric materials by evaluating Seebeck coefficients. The primary objective was to optimize the thermoelectric leg materials, specifically Cu_2Te, $Cu_2BiSbTe$, and $Cu_2Bi_2Te_3$, for enhanced performance in thermoelectric generators like [6]. The simulations were carried out by modelling temperature and electrical potential distributions in TMLs and analyzing how various factors such as material properties, temperature, thermoelectric leg height, and cooling mechanisms affect device efficiency. The simulations employ the Heat Transfer Module with stationary analysis. The results showed that $Cu_2Bi_2Te_3$ exhibited superior thermoelectric performance when compared to the other materials tested. The Seebeck coefficient of $Cu_2Bi_2Te_3$ was found to be 141 μV/K, which is significantly higher than that of $Cu_2BiSbTe$ (84 μV/K) and Cu_2Te (47 μV/K). These findings are in agreement with the experimental data available for materials at temperatures below 560 K, demonstrating that $Cu_2Bi_2Te_3$ is particularly effective at higher temperatures, thus making it an ideal material for high-performance thermoelectric legs [4, 31]. Thermoelectric effects are incorporated through iso-thermal flow multiphysics interface [25, 31]. The governing equations account for heat conduction, convective cooling, electric currents, Joule heating, and thermoelectric coupling. Table 1 represents the simulation results; it shows that $Cu_2Bi_2Te_3$ exhibits the highest electric potential among the investigated materials, which is consistent with reported experimental data below 560 K [9]. With heat sink cooling applied and an inlet temperature of 298.25 K, $Cu_2Bi_2Te_3$ produces an electric potential approximately 24% higher than $Cu_2BiSbTe$ at 450 K. At 615 K, the electric potential is about 20% higher when temperature dependent material properties are used. Heat transfer efficiency reaches highest for $Cu_2Bi_2Te_3$ and Cu_2Te due to their lower thermal conductivities [4].

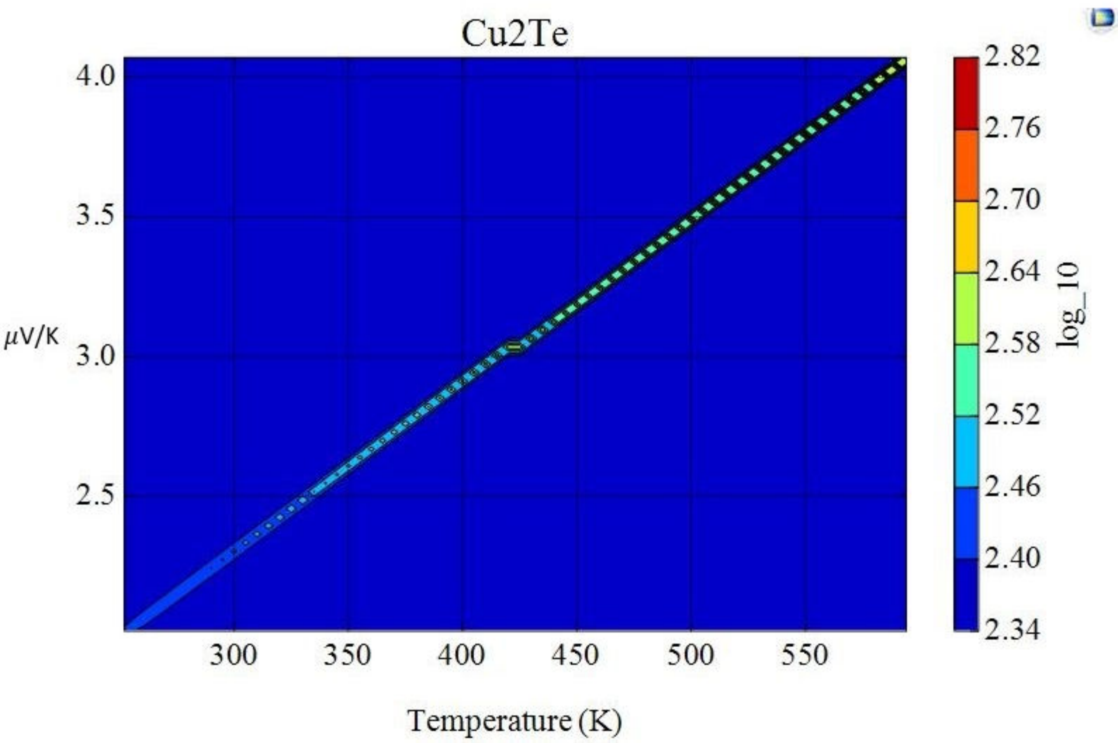

Figure 3. Seebeck Coefficient of Cu_2Te .

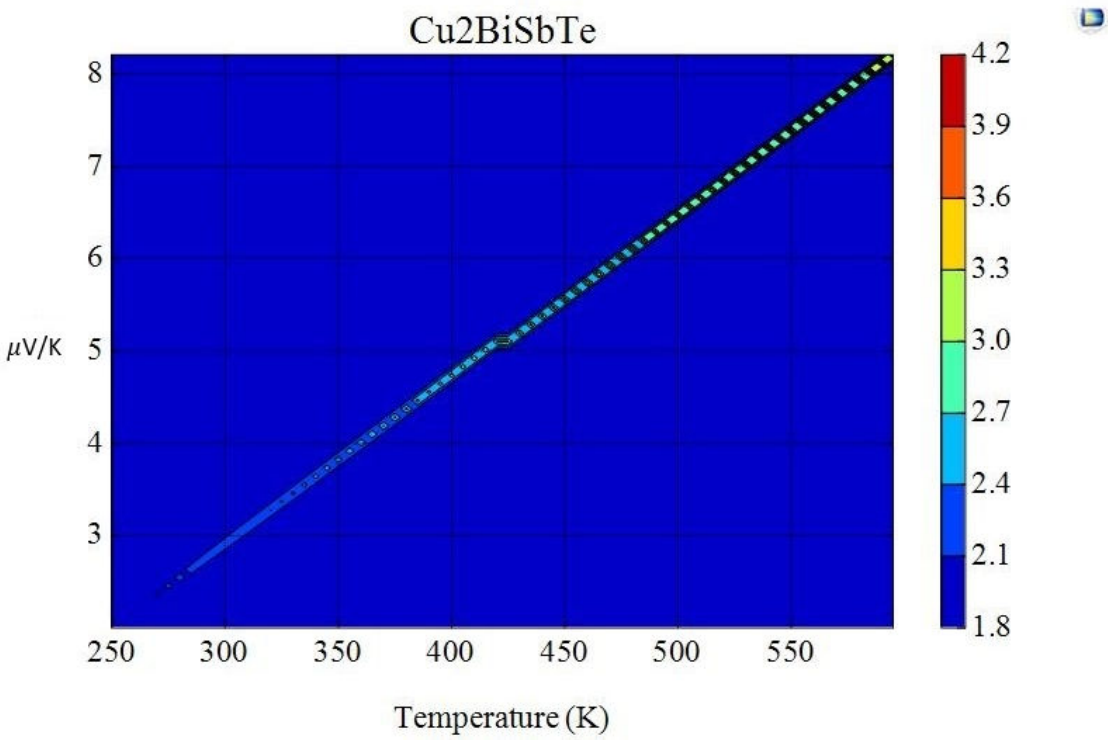

Figure 4. Seebeck Coefficient of $Cu_2BiSbTe$.

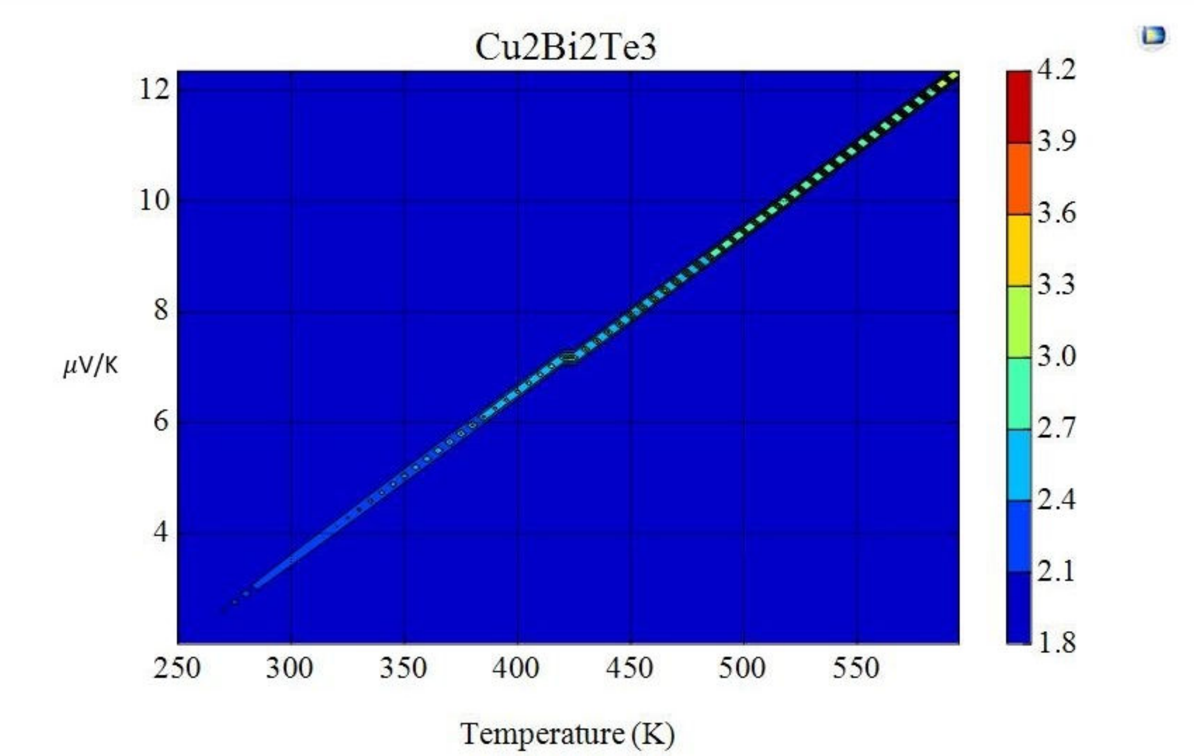

Figure 5. Seebeck Coefficient of $Cu_2Bi_2Te_3$.

Table 1. Output obtained for thermoelectric materials: Cu_2Te, $Cu_2BiSbTe$ and $Cu_2Bi_2Te_3$.

Simulation Output	**Cu_2Te**	**$Cu_2BiSbTe$**	**$Cu_2Bi_2Te_3$**
Seebeck Coefficient	47 μV/K	84μV/K	141μV/K
Electric potential	5081 S/cm	5482 S/cm	5782 S/cm
Thermal conductivity	3.123 W/cm.K^{-1}	3.152 W/cm.K^{-1}	3.206 W/cm.K^{-1}

4. CONCLUSION

A COMSOL based 3D model was developed to enhance TML efficiency by considering thermoelectric materials. $Cu_2Bi_2Te_3$ demonstrates superior thermoelectric performance, with a Seebeck coefficient of 141 µV/K and enhanced electric potential at elevated temperatures. The results confirm that accurate temperature dependent material properties are essential for a reliable thermoelectric modelling. The electric potential was computed for various thermoelectric materials at different temperatures, considering the effects of heat sinks and inlet temperatures. At 450 K, $Cu_2Bi_2Te_3$ produced an electric potential approximately 24% higher than $Cu_2BiSbTe$, and at 615 K, the calculated electric potential was about 20% higher than that obtained with temperature dependent physical constants. These improvements were particularly notable when comparison is done to the behaviour of the materials without incorporation of accurate temperature dependent properties. One of the key findings of the simulations was the role of thermal conductivity in overall performance of thermoelectric materials. $Cu_2Bi_2Te_3$ and Cu_2Te demonstrated the highest heat transfer efficiency due to their relatively lower thermal conductivities compared to $Cu_2BiSbTe$. This reduced thermal conductivity allows a more efficient temperature gradient across the thermoelectric legs, leading to improved power generation.

5. FUTURE SCOPE

The simulations also revealed that segmented thermoelectric legs outperformed non-segmented configurations. By using a segmented approach, different materials optimized for various temperature ranges could be used, thereby enhancing overall efficiency of the thermoelectric generator. However, it is important to note that interface resistance between the segments could reduce the electrical conductivity, and it needs to be optimized in future designs.

- Material Selection: $Cu_2Bi_2Te_3$ is the most promising material for thermoelectric legs due to its superior Seebeck coefficient and electric potential generation capabilities. The material's performance is further enhanced at elevated temperatures (above 450 K), making it suitable for high temperature applications.
- Temperature Dependence: Accurate temperature dependent material properties are critical for reliable modelling. The simulation results confirmed that using these properties in the model led to more accurate predictions, particularly at higher temperatures (615 K), where the material behaviour deviates from the constant values traditionally used in thermoelectric simulations.
- Cooling Systems: The incorporation of cooling mechanisms, such as heat sinks and fluid coolers, improves the efficiency of thermoelectric devices by maintaining a low cold-side temperature, which is crucial for maximizing the temperature difference across the thermoelectric legs.
- Further Research: Future studies should focus on identifying additional nanomaterials that can offer improved efficiency and cost-effectiveness. Moreover, optimizing the geometry and materials of cooling systems and heat sinks will be essential to enhance device performance further.

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