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The Thermoelectric Optimization Of Bismuth Telluride At 300K

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Abstract - This project explores the thermoelectric properties of Bismuth Telluride (Bi_2Te_3) at 300 K, with the aim of finding the highest possible figure of merit (ZT) by optimizing key material parameters. The goal is to assess how an optimized sample of Bi_2Te_3 could be used in real thermoelectric devices. Using a simulation that includes realistic values for band structure and scattering properties from experimental data, we predicted how ZT changes under different conditions. In this project we focused on improving thermoelectric efficiency by adjusting parameters like carrier concentration, while keeping the band structure close to that of the real material. Our results matched well with published values, suggesting the simulation is reliable. We then tested how far ZT could be improved by increasing carrier concentration and found an optimal range that agreed with values reported in the literature. Finally, the simulation was extended to include possible effects from advanced manufacturing techniques and nanoscale engineering, to see if ZT could be increased further. Overall, this project highlights the key factors that affect the thermoelectric performance of (Bi_2Te_3) and shows how simulation-based optimization can help guide future improvements in material design.

Keywords - Bismuth Telluride; Thermoelectric Materials; Figure of Merit; Carrier Concentration; Material Optimization

1 Introduction

1.1 Historical Context

The ability of certain thermoelectric materials to transform typically wasted heat into a usable electricity source has been a focus of many material scientists for decades. Bismuth Telluride (Bi₂Te₃) is one of the most commonly used materials in thermoelectric generators (TEGs) and Peltier cooling devices due to its relatively high efficiency near room temperature. Compared to other semiconducting materials such as Bismuth Selenide Bi₂Se₃, Bi₂Te₃ can convert heat into electrical energy more effectively, making it a strong candidate for energy harvesting applications. Its dimensionless figure of merit, *ZT*, typically ranges from 0.5 to 1.5 at 300 K, depending on fabrication techniques. For instance, nanostructuring and doping with group 15 elements such as Antimony (Sb) have been shown to enhance its thermoelectric performance [1]. Additionally, direct measurement techniques such as the Harman method have been employed to more accurately determine the *ZT* value of Bi₂Te₃ samples [2]. This makes Bi₂Te₃ well-suited for thermoelectric applications. One crucial advantage is that since Bi₂Te₃ can operate at room temperature, this gives a strategic advantage of using needing a minimal amount of energy into a Bi₂Te₃ based thermoelectric device (TED) system or to take small amounts of energy out before we note a desirable level of thermoelectric performance from Bi₂Te₃. The development of efficient room-temperature semiconducting materials has been a major focus within the scientific community, as devices operating near ambient conditions generally exhibit greater stability and longevity compared to those functioning at elevated temperatures. Additional advantages include the sustainability and relatively low cost of such materials, particularly in the case of Bismuth Telluride (Bi₂Te₃), which is already widely adopted in commercial thermoelectric applications. These factors make the investigation of Bi₂Te₃'s thermoelectric performance at room temperature especially relevant. Understanding and optimizing its behavior under these conditions contributes to the broader goal of improving the efficiency and viability of thermoelectric materials for practical energy conversion technologies.

The figure of merit (ZT) for a thermoelectric material is given by:

$$ZT = \frac{S^2 \sigma T}{\kappa} \tag{1}$$

where:

- *S* is the Seebeck coefficient (Volts per Kelvin, V/K).
- σ is the electrical conductivity (Siemens per Meter, S/m).
- *T* is the absolute temperature (Kelvin, K).
- κ is the total thermal conductivity (Watts per Meter per Kelvin, W/(m·K)), which consists of two components:

$$\kappa = \kappa_e + \kappa_l$$

where κ_e is the electronic thermal conductivity, and κ_l is the lattice (phonon) thermal conductivity.

These parameters are used to analyze the thermoelectric efficiency of the material and then this allows researchers to evaluate whether the material has an appropriate figure of merit (FOM) to then consider manufacturing the material to be applied into TED's.

Maximizing *ZT* is difficult due to the reciprocal dependencies within the equation. For example, increasing the carrier concentration *n* improves the electrical conductivity σ , but reduces the Seebeck coefficient *S*, since $S \propto 1/n$ while $\sigma \propto n$. Furthermore, increasing σ also increases the electronic thermal conductivity κ_e through the Wiedemann-Franz law: $\kappa_e \propto \sigma T$. This results in a frustrating trade-off where enhancing one part of the equation negatively affects another, making it a crucial point of research to optimize all parameters simultaneously. Furthermore, *ZT* typically reaches a maximum at an intermediate carrier concentration which balances the equation, giving us an advantage of having a unique carrier concentration that yields the best thermoelectric performance for Bi₂Te₃.

It is crucial to understand the principles that influence the thermoelectric properties of Bi_2Te_3 and its alloys, which enhance their performance. Generally, the uses of solid-state TEGs are for very niche, highly specialized applications, an example of this would be space probes. Using heat sources provided by decaying radioactive isotopes they can be converted into electricity. For example, Rover 1 which was launched in 1977 is still powered today because of thermoelectric generators that convert that heat from radioactive decay into a usable electricity source. To calculate a thermoelectric devices efficiency we use the following equation

$$\eta = \frac{\Delta T}{T_{\text{hot}}} \cdot \frac{\sqrt{1 + Z\bar{T}} - 1}{\sqrt{1 + Z\bar{T}} + \frac{T_{\text{cold}}}{T_{\text{hot}}}}$$
(2)

where:

 η is the efficiency of the thermoelectric device.

 ΔT is the temperature difference between the hot and cold sides $T_{hot} - T_{cold}$.

 T_{hot} is the absolute temperature of the hot side (Kelvin).

 T_{cold} is the absolute temperature of the cold side (Kelvin).

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Z is the figure of merit of the thermoelectric material (units of inverse temperature).

 \overline{T} is the average temperature, defined as $\frac{T_{\text{hot}}+T_{\text{cold}}}{2}$.

The operation of TEGs relies on the Seebeck effect, which states that a temperature gradient across two different materials induces a voltage, driving an electric current that can be utilized for power generation.

The Seebeck voltage *V* generated is given by:

$$V = S \Delta T = S(T_{\text{hot}} - T_{\text{cold}})$$
(3)

where:

V is the voltage generated by the temperature difference.

S is the Seebeck coefficient (Volts per Kelvin, V/K).

 ΔT is the temperature difference, $T_{\text{hot}} - T_{\text{cold}}$ (Kelvin).

 T_{hot} is the absolute temperature of the hot side (Kelvin).

 T_{cold} is the absolute temperature of the cold side (Kelvin).

It is challenging to replicate the same temperature gradient in TEG when they are to be used in everyday personal technology. Replicating the amount of electricity put out from a corresponding heat source in devices at much lower temperatures, such as room temperature, has proved to be difficult. Modifications to the band structure of the material and the scattering properties are necessary to optimize Bi₂Te₃.

Bi₂Te₃ is typically alloyed with materials from group 15, such as Antimony (Sb) this allows us to maintain similar crystallographic structure and maintain electrical conductivity properties. For this purpose, Bi_{0.5}Sb₁Te₃ is a common alloy that demonstrates a significant improvement in its figure of merit compared to bulk Bi₂Te₃, making these alloys more promising for applications [3].

The following simulations focuses on p-type extrinsic Bi_2Te_3 , with a discussion of its alloys and an investigation into the limitations of its thermoelectric performance. We are inferring that the Bi_2Te_3 is extrinsic and p-type due to natural structural defects produced in Bi_2Te_3 and that the predominant carrier in the simulation was holes. We will be investigating results through simulation so some values compared to real world lab replication will have some error. What this paper aims to do is to create the highest ZT possible for our Bi_2Te_3 simulated sample at a constant 300 K and also provide further insight into optimization of thermoelectric parameters which effect the figure of merit.

1.2 Previous Studies

It has been well known that the rough ZT for p-type Bi₂Te₃ is around 1 to 1.3, depending on small alloys introduced into Bi₂Te₃ [4]. In this study they were able to increase the thermoelectric performance of p-type Bi₂Te₃ through alloying it with Antimony and using hot deformation which essentially added small microstructures to their crystal of Bismuth Antimony Telluride. As a result of their work they were able to achieve a ZT of 1.3 and was achieved at a temperature 380K. The best figure of merit for a p-type Bi₂Te₃ alloy achieved was a value of 2.4. This significant enhancement was achieved using p-type Bi₂Te₃/Sb₂Te₃ super-lattice structures [5]. In this material, thin alternating layers of Bismuth Telluride and Antimony Telluride are stacked to form a repetitive structure. This super-lattice design reduced the lattice thermal conductivity by scattering phonons between the layers of the material, which allowed them to maintain electrical conductivity.

In [5] study, the researchers also manufactured quantum wells within the bands of their samples to optimize the behavior of the charge carriers. By designing quantum wells to concentrate the majority of the charge carriers into small conductive regions, the regions surrounding these quantum wells by contrast, were less conductive. This resulted in a supper-lattice structured alloy of Bi₂Te₃ where charge carrier activity was primarily focused within the quantum well regions. The result is a substantial increase in the figure of merit, making these super-lattice structures highly efficient for

thermoelectric applications. An important point to add is that when their research was conducted that the temperature they used was much higher then room temperature value which was at 380 K, around 106° Celsius. We will explain their motivation for this specific temperature choice when we model ZT as a function of its temperature and carrier concentration in section 3.3.

2 Methodology

2.1 Simulation Choice

One challenge that occurred immediately was that there was no individual place in current literature that stated the values needed for the simulation for Bi₂Te₃. Relevant data were obtained through cross-referencing multiple studies. Secondly, We were careful to make sure that from the cited literature that these sources did not make fundamental changes to the crystal structure of Bi₂Te₃ as to make sure our results were consistent for bulk Bi₂Te₃ which by default still has minor defects in its crystallography. A tool on Nanohub.org was used to condone this project [6]. Which allowed us to input custom band structures and input scattering properties into the simulation using the linearized Boltzmann Transport Equation.

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \mathbf{F} \cdot \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \tag{4}$$

Equation (4) is the Boltzmann transport equation (BTE). It describes how the distribution function $f(\mathbf{r}, \mathbf{k}, t)$ evolves due to external forces and collisions.

$$f(\mathbf{r}, \mathbf{k}, t) = f_0(\mathbf{k}) + g(\mathbf{r}, \mathbf{k}, t), \quad \text{with } g \ll f_0$$
(5)

In Equation (5), you can linearize the distribution function around the equilibrium Fermi-Dirac distribution $f_0(\mathbf{k})$.

$$\mathbf{v} \cdot \nabla_{\mathbf{r}} f_0 + \mathbf{F} \cdot \nabla_{\mathbf{k}} f_0 = -\frac{g(\mathbf{r}, \mathbf{k}, t)}{\tau}$$
(6)

Equation (6) is obtained by substituting the linearized form (5) into the full BTE (4) and then applying the relaxation time approximation [7].

Variable definitions:

- *f*(**r**, **k**, *t*): Distribution function of charge carriers.
- $f_0(\mathbf{k})$: Equilibrium Fermi-Dirac distribution.
- $g(\mathbf{r}, \mathbf{k}, t)$: Deviation from equilibrium, $g \ll f_0$.
- **v**: Carrier velocity, $\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon(\mathbf{k})$.
- **F**: External force $\mathbf{F} = -e\mathbf{E}$ for an electric field).
- τ : Relaxation time (average time between scattering events).
- ∇_r : Gradient with respect to position.
- $\nabla_{\mathbf{k}}$: Gradient with respect to wavevector.
- $\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$: Collision term in the BTE.

It is very handy to have a calculator for (4) as quantitative calculations using (4) are time consuming and not within the scope of this paper.

Starting by inputting values from referenced sources and inferred quantities [8-11] into our simulation to see what our bulk p-type bismuth telluride would generate as its initial ZT. The full table of values used are attached in the appendix.

3 Results and Analysis

Firstly, as demonstrated from Figure 1, it appears that both ZT and the power factor ($S^2\sigma$) increase exponentially with carrier concentration. The peak ZT achieved by this simulation is 1.36, which occurred at a hole carrier concentration of 1×10^{19} cm⁻³, this agrees with current literature as p-type Bi₂Te₃ at 300 K typical ZT lies around 1.2 to 1.3 [12].

3.1 First Result



Figure 1: Simulation result at 300 K. Red Line: ZT vs concentration, Blue Line: Power Factor vs concentration

The carrier concentration in Figure 1 ranges from 1×10^{17} to 1×10^{19} cm⁻³, which is typical for bulk materials. For the next simulation, we decided to increase the carrier concentration by nearly two orders of magnitude to see if we could find the point where increasing the carrier concentration *n* reduces the Seebeck coefficient *S*, since $S \propto 1/n$ and $\sigma \propto n$.

3.2 Increasing Carrier Concentration

This next simulation shows a wider range of carrier concentrations ranging from 2×10^{17} to 8×10^{20} cm⁻³ which shows us a graph of our Bi₂Te₃ where the carrier concentration magnitudes of 10^{17} represents a bulk material of Bi₂Te₃, 10^{19} is a fairly doped version of Bi₂Te₃ and carrier concentrations of 10^{20} represent a very highly doped version of Bi₂Te₃. In Figure 2 the peak ZT was 1.73 which occurred a carrier concentration of 3.77×10^{19} cm⁻³.



Figure 2: Simulation with increased carrier concentration at 300 K. Red Line: ZT vs concentration. Blue Line: Power Factor vs concentration.

3.3 3D Representation of ZT as a function of carrier concentration and temperature

The previous two simulations led us to model ZT as a function of carrier concentration and temperature and so we wrote code to provide this.

As soon will be demonstrated in Figure 3, we completed a parametric study from 200 to 500 K. Each 25 increments in Kelvin had 24 unique carrier concentration points with another 24 unique ZT points which was calculated by the original software and then this data was inputted into a code so that we could produce this 3D representation of ZT as a function of carrier concentration and temperature. If you follow the data point at 300 K up and to the corresponding peak that is the representation of our initial simulation where ZT was 1.36. Secondly this graph can also show some motivation for a previous study [5] study and why they chose 380 K as to follow the new tail of exponential growth that occurs around 350 K on Figure 3. An important note is that this dataset only uses quantifying behavior meaning ZTs simulated at less than less than 10^{-2} (e.g. a ZT of 0.03) were emitted and given in the dataset as 0 due to limitations in the coding software. While this affects the distribution it does not affect the important information provided by the simulation.

ZT as a Function of Temperature and Carrier Concentration



Figure 3: ZT as a function of carrier concentration and temperature.

3.4 Increasing ZT further through parameter adjustments

To further increase ZT and maintain continuity from our simulated Bi_2Te_3 adjustments were made to our parameters in the simulation that would not dramatically affect the band structure of the material. Firstly we reduced the lattice thermal conductivity by 30% which we achieved by inferring we had Sb/Se alloying and increased the static dielectric constant to increase screening in the simulation. The static dielectric constant was increased from 100 to 150 [13,14]. Another adjustment included reducing deformation potentials from 10 eV for acoustic phonon deformation potential scattering to 7 eV and reduced our optical phonon deformation potential scattering from 15 eV to 7 eV [15,16]. These changes allowed us to replicate a Bi_2Te_3 alloy sample with some idealized adjustments to increase ZT.



Figure 4: New Simulated Bismuth Telluride with idealized adjustments (Red Line: ZT vs concentration at 300 K, Blue Line: Power Factor vs concentration at 300 K)

As shown, the introduction of our new parameters led to a remarkably high peak figure of merit

(ZT) of 4.26 at a carrier concentration of $1.57 \times 10^{19} \text{ cm}^{-3}$. This represents a 213.23% increase over our baseline simulation shown in Figure 2. While this result is encouraging from a theoretical standpoint, it significantly exceeds experimentally reported values for Bi₂Te₃ alloys, which typically peak around ZT $\approx 1-1.5$, with very few exceptional cases approaching 2.6 [5]. A ZT of 4.26 has not been demonstrated in laboratory settings or reported in literature, raising questions about the physical plausibility of this outcome. If this level of performance could be achieved experimentally, it would represent a major breakthrough in thermoelectric materials. However, the large gap between our simulated result and values reported in the literature suggests that our model may be idealized, potentially neglecting important physical limitations such as phonon scattering or boundary effects that would reduce efficiency in real materials.

3.5 Discussion of Results

As has been demonstrated in this paper the best carrier concentration for the highest ZT occurs within the magnitude of 10¹⁹ cm⁻³. This also agrees with current literature [17]. We started with a bulk Bi₂Te₃ material which gave an initial ZT of 1.36. Following this, the carrier concentration was increased to see how the increase in available carriers stopped assisting and showed where it negatively affects the Seebeck effect and consequently ZT. This was found to be around 3×10^{19} cm⁻³ from Figure 2 and was later confirmed by Figure 4 to be 1.57×10^{19} cm⁻³. While these values vary, the magnitude 10^{19} cm⁻³ is the optimal carrier concentration for Bismuth Telluride and its alloys when held at a constant 300 K. By inferring modifications to the crystallography and suggesting manufacturing processes that could further increase ZT represented in Figure 4. In summary there are challenges that would have to be faced to replicate the results shown in these simulations to lab results. These processes are beyond the time frame and scope of this project and will be explored in Chapter 4. The results generated in these simulations were promising as they agreed with current literature especially Figures 1,2 and 3. This shows that the simulation software has a potential to be used for foundational work for research groups before conducting the manufacturing of a Bi₂Te₃ sample for them to then test and make the sample efficient enough to be applied into thermoelectric devices namely TEG and Peltier coolers. The way to interpret these results at 300 K is to see this materials performance snippet as if it was inside a TEG or using the following equation to calculate the contribution of ZT at a given point, in this paper that was 300 K.

$$Z\bar{T} = \frac{1}{\Delta T} \int_{T_{\text{cold}}}^{T_{\text{hot}}} Z(T) T \, dT \tag{7}$$

where:

- Z(T) is the temperature-dependent figure of merit at absolute temperature T.
- *T* is the absolute temperature (in Kelvin).
- T_{hot} is the temperature of the hot side of the device (K).
- T_{cold} is the temperature of the cold side of the device (K).
- $\Delta T = T_{hot} T_{cold}$ is the temperature difference across the device (K).
- $Z\bar{T}$ is the average figure of merit over the temperature gradient.

4 Conclusion

4.1 Limitations

Firstly as stated within this paper, we are very aware of the idealized optimizations used when generating our simulation for Figure 4. One particular limit that made itself very apparent is that due to the simulation software format from [6] was that regardless of how we input values we could not simulate the crystal structure of this material which meant we had to infer and use assumptions to validate the theoretical crystal structures of materials simulated in Figures 1,2 and 4. While it was possible to infer the crystal structures of the materials simulated none of the papers cited explicitly

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listed the crystal structure or unit cells present for their material, so we could not account for where dislocations and voids occurred in our materials structure. We also could not accurately add ratios of Bismuth, Tellurium, Selenium or Antimony atoms into the simulation that we saw in Figure 4. While we could not implement this into the simulation rigorously we are fully aware that there are ideal ratios which are used in lab tests for these compounds which show an increase in ZT in comparison to lightly doped Bi_2Te_3 samples.

4.2 In Conclusion

In conclusion Bismuth Telluride is a very good material that can be applied to thermoelectric devices and can be optimized before being inputted into a thermoelectric device to ensure greater thermoelectric efficiency. While simulations suggest substantial ZT improvements, the absence of grain boundary scattering and fabrication constraints limit direct real-world applicability.

4.3 Future Work

This project demonstrates potential for future experimental work to be extrapolated onto fabricating a Bi₂Te₃ sample. The results shown in these simulation should encourage research groups to do further research on the material. Another advantage to be utilized is using multiple pieces of simulation software to further enhance our understanding of the results found in this paper and be 100 % confident that the results found in this simulation could be produced in a real lab. We could also decide on fabrication processes and do very specific processes like adding thin films to make phonons scatter between layers of our material to reduce the thermal phonon conductivity. Nanostructures being introduced also show a great improvement on the ZT of Bi₂Te₃ in lab as demonstrated in [5]. The ideas expressed in the referenced papers show manufacturing methods to increase ZT on Bi₂Te₃ in a lab setting. While we were not able to confirm the best ZT achievable for Bi₂Te₃ at 300 K, this paper provides a foundation for future researchers for the optimal ranges for ZT and as a function of carrier concentration extrinsic p-type Bi₂Te₃ semiconductors to refer too. This will allow future researchers to use our established basis to begin their work.

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