BASIC PARAMETERS OF THERMOELECTRIC MATERIALS

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Abstract: Thermoelectric materials have gained significant attention due to their ability to directly convert heat into electrical energy and vice versa. The performance of these materials is primarily determined by three key parameters: the Seebeck coefficient (S), electrical conductivity (σ), and thermal conductivity (κ). The interplay among these parameters defines the dimensionless figure of merit, $ZT = S^2\sigma T/\kappa$, which serves as a standard metric for evaluating thermoelectric efficiency. Optimizing ZT requires balancing high electrical conductivity and Seebeck coefficient with low thermal conductivity. Advanced strategies such as doping, band structure engineering, and nanostructuring have been developed to enhance carrier mobility and suppress phonon transport. Materials like PbTe, SiGe alloys, and Bi-Te based compounds have demonstrated excellent thermoelectric performance, particularly at medium to high temperatures. Anisotropic crystal structures and tailored microstructures also contribute significantly to improved energy conversion. This study reviews the physical and structural factors that influence thermoelectric properties, and highlights the potential of thermoelectric materials for applications in energy harvesting, space exploration, and electronic cooling systems.

Key words: Thermoelectric materials, Seebeck coefficient (S), Electrical conductivity (σ), Thermal conductivity (κ), Power factor ($S^2\sigma$), Figure of merit (ZT), Energy band gap (Eg), Carrier concentration, Carrier mobility, Phonon scattering, Electron transport, Lattice thermal conductivity, Electronic thermal conductivity,

Doping (n-type / p-type), Band engineering, Anisotropy, Nanostructuring, Thermoelectric generator (TEG), Thermoelectric cooling,

Introduction

The key parameters of thermoelectric materials are based on several important metrics that determine their properties and overall efficiency. These materials are used either to convert heat into electrical energy or to perform the reverse process. In addition, thermoelectric materials must meet specific requirements, such as high thermal stability, time-invariant thermoelectric power (TEP), a maximized value of TEP, and a monotonic relationship with temperature. Furthermore, they should exhibit a low temperature coefficient of resistance and high electrical conductivity. Below is a comprehensive overview of the main parameters of thermoelectric materials.

Bismuth telluride (Bi_2Te_3) is primarily used in the low-temperature range (0–200°C). It has a rhombohedral trigonal crystal structure and a narrow band gap of approximately 0.15 eV. Its electrical conductivity ranges between 10^3 and 10^4 S/m, and it exhibits very low thermal conductivity (~1.5 W/mK), which is advantageous for thermoelectric efficiency. Bismuth telluride is the most widely used thermoelectric material for low-temperature applications, typically operating within the 200 K to 400 K range (i.e., room temperature and slightly above). The Seebeck coefficient is approximately –200 μV/K for n-type and +200 μV/K for p-type materials. The figure of merit (ZT) typically lies in the range of 1–1.2 at 300 K, and it can reach up to 1.5 in specially engineered Bi_2Te_3-based materials.

The primary factors contributing to thermoelectric performance include low thermal conductivity (especially due to the minimal contribution of lattice phonons), high electrical conductivity, and a large Seebeck coefficient—enabling significant voltage generation under a temperature gradient. The atomic structure of Bi_2Te_3 is layered, composed of Te–Bi–Te–Bi–Te quintuple layers bonded by

weak Van der Waals forces. This layered structure results in pronounced anisotropic properties, with electrical and thermal conductivities differing along various crystallographic directions.

Bismuth telluride is widely used in thermoelectric cooling devices (e.g., Peltier elements), waste heat recovery (e.g., in automotive systems), portable cooling systems, microelectronic device cooling, and power supply units in space technology, such as in radioisotope thermoelectric generators (RTGs).

Enhancement of the thermoelectric performance of Bi_2Te_3 is often achieved through alloying. Typically, selenium is used for n-type doping and antimony for p-type doping. Nanostructuring techniques, which scatter phonons and reduce lattice thermal conductivity, are also employed to improve efficiency. Today, Bi_2Te_3 remains one of the most efficient low-temperature thermoelectric materials due to its high ZT values and favorable electrical and thermal properties. Its layered crystal structure and narrow band gap make it ideally suited for thermoelectric applications. Future improvements in device performance are expected through nanoscale engineering approaches in Bi_2Te_3-based materials.

PbTe has a cubic NaCl-type (rocksalt) crystal structure, characterized by a face-centered cubic (FCC) lattice. Its band gap energy is approximately 0.31 eV, and it demonstrates moderately high electrical conductivity in the range of 10^3–10^4 S/m. At 300 K, the thermal conductivity is relatively low (~2 W/m·K), which is favorable for thermoelectric performance. Uniquely, PbTe exhibits an increasing band gap with rising temperature, a behavior that is opposite to that of most semiconductors.

PbTe is considered one of the most effective thermoelectric materials for the mid-temperature range of 450–800 K. Its Seebeck coefficient is around +200 to +300 μV/K for p-type, and approximately –200 μV/K for n-type material. The

figure of merit (ZT) reaches values of 1.0–1.5 at 700–800 K in optimally doped and structurally engineered samples.

The high thermoelectric efficiency of PbTe stems from its high electrical conductivity, low lattice thermal conductivity, and temperature-dependent band gap, which collectively enhance performance. Moreover, carrier concentration control through doping plays a crucial role. By introducing suitable dopants, the carrier concentration can be optimized to approximately $10^{19}\,cm^{-3}$, while band degeneracy (i.e., multiple energy valleys) contributes to increased charge carrier mobility.

Experimental studies have shown that PbTe crystals are typically grown using advanced techniques such as solution growth or self-flux methods. Doping with elements like Na, K, Cl, or Bi enables the fabrication of high-performance p-type and n-type PbTe. At room temperature, PbTe has a thermal conductivity of 2–3 W/m·K, a Seebeck coefficient of around +250 μV/K, and a ZT of approximately 0.8. With optimal doping at 750 K, ZT values of 1.4–1.5 can be achieved.

These results have been validated in thermoelectric generators based on PbTe, particularly in automotive waste heat recovery systems and radioisotope thermoelectric generators (RTGs) used in spacecraft.

Advanced approaches like nanostructuring—embedding nanoparticles within the PbTe crystal lattice—further reduce phonon transport, lowering thermal conductivity. Techniques such as band convergence enhance both the Seebeck coefficient and electrical conductivity simultaneously. Additionally, supervoid structures (nano-voids within the crystal) have been shown to significantly suppress thermal conductivity.

PbTe remains one of the most studied and efficient mid-temperature thermoelectric materials. Its high electrical conductivity, low phonon thermal

conductivity, and temperature-dependent band structure make it a key material for waste heat recovery, cooling systems, and space power technologies. Recent advancements in nanostructured PbTe materials are paving the way for next-generation energy-efficient thermoelectric technologies [1-3].

Silicon–germanium (SiGe) alloys are considered among the most promising materials in modern semiconductor technologies and thermoelectric devices. They are widely used due to their ability to maintain stable physical and electrical properties at elevated temperatures (800 K and above). These alloys play a critical role in high-temperature transistors, infrared detectors, thermoelectric generators, and aerospace systems.

SiGe alloys exhibit excellent thermal stability under high-temperature conditions. Their thermal conductivity is significantly lower compared to pure silicon, which is a major advantage for enhancing thermoelectric efficiency. Increasing the germanium content further reduces thermal conductivity. For example, SiGe alloys containing 20–30% Ge retain low thermal conductivity in the 800–1200 K temperature range, thereby protecting devices from overheating and extending their operational lifespan. The thermal expansion coefficient of SiGe alloys can also be precisely controlled. As the germanium concentration increases, the alloy's expansion also increases, which is crucial for ensuring material compatibility in high-temperature applications. SiGe alloys are among the most efficient materials for high-temperature thermoelectric devices. Their Seebeck coefficient is relatively high and increases with temperature. The combination of good electrical conductivity and low thermal conductivity enables SiGe alloys to achieve a high thermoelectric figure of merit. Through doping (e.g., with boron for p-type or phosphorus for n-type), the electrical conductivity and Seebeck coefficient of SiGe alloys can be optimized, further enhancing thermoelectric performance.

At temperatures of 800 K and above, thermoelectric elements based on SiGe alloys are capable of efficiently generating electrical energy. SiGe-based thermoelectric modules are primarily used in space probes and other aerospace applications, where long-term reliability and high-temperature performance are essential [4-5].

The physical structure, particularly the crystal structure and layer arrangement of a material, significantly affects its thermoelectric properties. Suitable crystal structures—such as nanocrystalline architectures—enable control over electron transport and efficient heat dissipation, both of which are critical for improving thermoelectric performance. Optimizing the physical structure of a material can lead to a considerable enhancement in its thermoelectric efficiency. To achieve high performance, it is essential to balance all contributing parameters and utilize them in an optimal way. With the development of new materials and technologies, thermoelectric characteristics can be further improved, making these materials applicable in energy, automotive, electronics, and other industries.

A diagram of a thermocouple element is shown in Figure 1. A thermocouple consists of two branches. These branches are made from materials with non-zero and typically opposite thermoelectric coefficients (α_n and α_p). In such a configuration, the electromotive forces (EMFs) generated in each leg add together.

This is the classical model of a thermocouple element, which is widely used in practice and well understood. In a thermocouple circuit, a non-homogeneous medium is employed: while each leg of the thermocouple is made of a homogeneous material, inhomogeneity occurs at the junction points where the legs are connected via commutation plates [6-9].

If the ends of the thermocouple legs are maintained at different temperatures, an electromotive force (EMF) arises across the open circuit due to the Seebeck effect. When the circuit is closed, an electric current flows through it. The

commutation plates themselves have negligible thermoelectric coefficients. Additionally, because the temperature at each plate is stable and uniform, their influence on the total EMF is minimal.

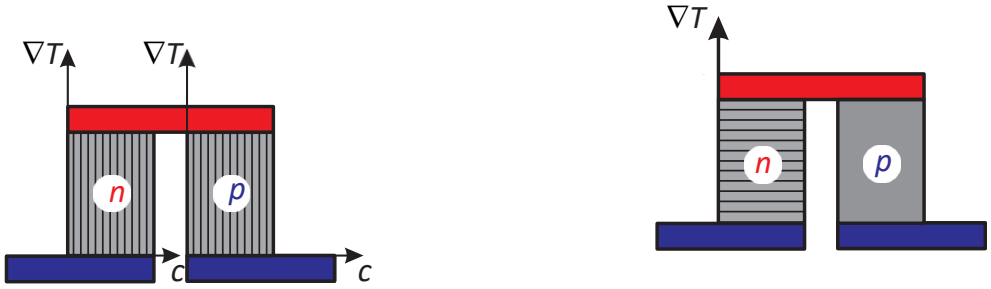
However, this model is only valid when the thermocouple legs are much longer than the carrier and phonon diffusion lengths at the contact points. If this condition is violated—for example, in the case of very small-scale thermocouples—then the overall EMF may become directly dependent on the materials of the commutation plates. In such cases, the classical model may no longer be applicable [10-15].

Thermocouple branches are often made from materials with crystalline structures. Such materials may exhibit anisotropy in physical properties, meaning their behavior can vary depending on spatial orientation. For example, both the thermoelectromotive force coefficient (Seebeck coefficient) and electrical conductivity can change based on the direction. Therefore, in such cases, the crystallographic axes of thermocouple branches are aligned relative to each other in a manner that maximizes energy conversion efficiency.

For instance, bismuth-tellurium (Bi-Te)-based thermoelements and their alloys are widely used. In such materials, the trigonal axis is typically oriented perpendicular to the temperature gradient. On the other hand, in bismuth-antimony (Bi-Sb)-based materials, the trigonal axis is aligned parallel to the temperature gradient (see Figure 1).

Research [16-17] has shown that the existence of thermoelectromotive force was first observed by Alessandro Volta. The idea of using this force to convert heat into electrical energy was initially proposed by Hans Christian Orsted. Therefore, from a historical standpoint, it would be more appropriate to refer to such elements as Volta-Orsted thermoelements.

When a thermocouple operates in a cooling or thermal heating mode, it is typically referred to as a Peltier thermoelement [18-20]. This naming corresponds with the physical phenomenon being exploited. However, historical records indicate that Jean Charles Athanase Peltier did not study his effect for the purposes of heating or cooling. The first practical applications in this domain were carried out by Heinrich Lenz in 1838. Therefore, it has been proposed that thermocouple elements used for cooling or heating be referred to as Peltier-Lenz thermoelements [21-24].



а) б)

Figure 1 Thermocouple Branches Made from Anisotropic Crystals

a) Thermocouple based on Bi-Te alloys: the trigonal c-axis is oriented perpendicular to the temperature gradient ∇T.

b) Thermocouple based on Bi-Sb alloys: the trigonal c-axis is oriented parallel to the temperature gradient ∇T.

Conclusion

These types of thermocouples are specifically designed for situations where high-performance thermoelectric materials are not available for both branches, but at least one efficient material is present. Such thermoelectric elements were first

used in practice in the late 19th and early 20th centuries by various inventors and developers of thermoelectric generators.

In these thermoelectric generators, one branch (the active branch) was typically made from materials like Zn-Sb (zinc-antimony) alloys, while the other (the passive branch) was made from iron or its alloys. Although the thermoelectromotive force (Seebeck coefficient) of iron or similar metals is relatively low, they still contribute somewhat to the total EMF of the thermopile. Hence, the term “passive” is relative in this context.

A clearer example of a true passive branch would be a thermocouple made from a superconducting material. Such thermocouples are designed to operate at very low temperatures, typically in the range of 120–150 K or below.

References

1. Khamidillaevich, Y. A. (2023). PARAMETERS OF OPTOELECTRONIC RADIATORS AND SPECTRAL CHARACTERISTICS IN DIFFERENT ENVIRONMENTS. *Journal of Integrated Education and Research*, *2*(4), 81-86.

2. Халилов, М. Т., & Юсупов, А. Х. (2023). МАКСВЕЛЛНИНГ УЗЛУКСИЗЛИК ТЕНГЛАМАСИНИНГ БАЁН ҚИЛИШ УСУЛИ. *Journal of Integrated Education and Research*, *2*(4), 77-80.

3. Xamidullayevich, Y. A., & Xalimjon o'g, T. N. Z. (2023). O ‘ZBEKISTON SHAROTIDA SHAMOL ELEKTR STANSIYALARINI O ‘RNATISH IMKONIYATLARI. *Journal of new century innovations*, *25*(1), 27-29.

4. Юсупов Абдурашид Хамидиллаевич, & Хамдамова Наргизой Хамидуллаевна. (2024). ЭЛЕКТРОМАГНИТ ИНДУКЦИЯ МАВЗУСИНИ ИНТЕРФАОЛ МЕТОДЛАР БИЛАН ЎҚИТИШ. *PEDAGOGS*, *48*(1), 43–50. Retrieved from https://pedagogs.uz/index.php/ped/article/view/575

5. Olimov, L. O., & Yusupov, A. K. (2021). The Influence Of Semiconductor Leds On The Aquatic Environment And The Problems Of Developing Lighting

Devices For Fish Industry Based On Them. *The American Journal of Applied Sciences*, *3*(02), 119-125.

6. Xalilov, M. T., & Yusupov, A. K. (2022). THE METHOD OF EXPRESSING MAXWELL'S EQUATIONS IN AN ORGANIC SERIES ACCORDING TO THE RULES, LAWS AND EXPERIMENTS IN THE DEPARTMENT OF ELECTROMAGNETISM. *European International Journal of Multidisciplinary Research and Management Studies*, *2*(10), 09-15.

7. Юсупова, У. А., & Юсупов, А. Х. (2022). ЎЗГАРМАС ТОК ҚОНУНЛАРИ БЎЛИМИНИ ЎҚИТИЛИШИДА НАМОЙИШ ТАЖРИБАСИНИНГ ЎРНИ. *PEDAGOGS jurnali*, *17*(1), 210-214.

8. Olimov Lutfiddin Omanovich, Akhmedov Alisher Khamidovich, & Yusupov Abdurashid Khamidillaevich. (2022). SCHEME OF HIGH VOLTAGE GENERATION USING SEMICONDUCTOR TRANSISTORS. *European Scholar Journal*, *3*(5), 42-49. Retrieved from https://scholarzest.com/index.php/esj/article/view/2206

9. Юсупов Абдурашид Хамидуллаевич, & Турсунов Навроз. (2023). ИСПОЛЬЗОВАНИЕ ЭНЕРГИИ ВЕТРА В МИРЕ И В УЗБЕКИСТАНЕ . *ОБРАЗОВАНИЕ НАУКА И ИННОВАЦИОННЫЕ ИДЕИ В МИРЕ*, *22*(2), 83–86. Retrieved from https://newjournal.org/01/article/view/6797

10. Abdurashid Khamidillayevich Yusupov Associate professor, Andijan machine-building institute, Uzbekistan. (2023). THE METHOD OF EXPLANATING THE ELECTROMAGNETIC INDUCTION PHENOMENON. Zenodo. https://doi.org/10.5281/zenodo.10201792

11. Yusupov Abdurashid Xamidullayevich, & Qodiraliyev Nursaid Botirali o`g`li. (2024). QUYOSH SPEKTRI VA FOTOELEKTRIK MATERIALINING YUTILISH SPEKTRI O‘RTASIDAGI NOMUVOFIQLIKNING TA’SIRINI KAMAYTIRISH. *Лучшие интеллектуальные исследования*, *14*(2), 64–71. Retrieved from http://web-journal.ru/index.php/journal/article/view/2891

12. Yusupov Abdurashid Khamidullayevich, & Artikov Dilshodbek Khushbaqjon ogli. (2024). PHOTOVOLTAIC EFFECTS AND THEIR EFFECTIVE USE. *Лучшие интеллектуальные исследования*, *14*(2), 21–27. Retrieved from http://web-journal.ru/index.php/journal/article/view/2884

13. Yusupov Abdurashid Xamidullayevich, & Yuldasheva Saodatkhan Sultanbek kizi. (2024). PPLICATION OF PHOTOVOLTAIC EFFECTS TO ENERGY-SAVING MATERIALS COMPONENTS OF THE STRUCTURE AND SOLAR CELLS. *Лучшие интеллектуальные исследования*, *14*(2), 105–109. Retrieved from http://web-journal.ru/index.php/journal/article/view/2897

14. Yusupov Abdurashid Khamidillaevich, & Yuldasheva Saodatkhon Sultonbek kizi. (2024). APPLICATION OF PHOTOVOLTAIC EFFECTS TO ENERGY SAVING MATERIALS. *Лучшие интеллектуальные исследования*, *21*(2), 62–68. Retrieved from https://web-journal.ru/journal/article/view/5316

15. Yusupov Abdurashid Khamidullayevich, & Khakimov Ulugbek ogli. (2024). DEVICES COLLECTING SUNLIGHTS. *Лучшие интеллектуальные исследования*, *21*(1), 193–199. Retrieved from https://web-journal.ru/journal/article/view/5297

16. Yusupov Abdurashid Khamidullayevich, & Rozmamatov Oybek Dilshodbek ogli. (2024). OBTAINING ELECTRICAL ENERGY USING DEVICES COLLECTING SUNLIGHTS. *Лучшие интеллектуальные исследования*, *21*(1), 187–192. Retrieved from https://web-journal.ru/journal/article/view/5296

17. Yusupov Abdurashid Khamidillaevich, & Artikov Dilshodbek Xushbakjon ogli. (2024). APPEARANCE OF PHOTOVOLTAIC EFFECT IN POLYCRYSTAL SILICON BASED RECEIVER. *Лучшие интеллектуальные исследования*, *21*(1), 179–186. Retrieved from https://web-journal.ru/journal/article/view/5295

18. Khamidillaevich, Y. A., & Abdumalik, T. (2024). HIGH TEMPERATURE SOLAR CONCENTRATORS. *Лучшие интеллектуальные исследования*, *21*(1), 200-206.

19. Kodirov, D., Makhmudov, V., Normuminov, J., Shukuraliev, A., Begmatova, N., & Abdurashid, Y. (2024). Determination of the optimal angle for high efficiency of solar panels in Uzbekistan. In *E3S Web of Conferences* (Vol. 563, p. 01008). EDP Sciences.

20. Lutfiddin Omanovich Olimov, ., & Abdurashid Khamidillaevich Yusupov, . (2022). DETERMINATION OF EFFICIENT OPTICAL SOURCES OF AIR PROPAGATION FOR FISHERIES BIOPHYSICAL DEVICES. European International Journal of Multidisciplinary Research and Management Studies, 2(10), 1–8. Retrieved from https://inlibrary.uz/index.php/eijmrms/article/view/23357

21. Olimov, L. O., & Yusupov, A. K. (2021a). TEMPERATURE DEPENDENCE OF TRANSISTOR CHARACTERISTICS OF ELECTRIC SIGNAL AMPLIFICATION IN OPTOELECTRONIC DEVICES. Theoretical & Applied Science, 8, 169–171.

22. Yusupov, A. K. (2021). Creating a biophysical trapping device based on an optical radiation source with a light-emitting diode. ACADEMICIA: An International Multidisciplinary Research Journal, 1530-1536.

23. Olimov Lutfiddin Omanovich, Y. (2020). Problems Of Implementation Of Semiconductored Leds For Fishery Lighting Devices. The American Journal of Engineering and Technology, 189–196.

24. Oripova Dilnoza Karimjon kizi, & Yusupov Abdurashid Khamidillaevich. (2024). PHENOMENON OF PHOTO EFFECT IN SEMICONDUCTORS. *JOURNAL OF NEW CENTURY INNOVATIONS*, *67*(4), 132-137. https://scientific-jl.org/new/article/view/7623