



Cover Page



REVIEW OF THERMOELECTRIC PROPERTIES OF Bi₂Te₃

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Abstract

Bismuth telluride (Bi₂Te₃) is one of the most widely used thermoelectric materials because of its excellent performance near room temperature. It can directly convert heat into electrical energy through the Seebeck effect and can also produce cooling when an electric current passes through it (Peltier effect). Bi₂Te₃ has a high Seebeck coefficient, good electrical conductivity, and low thermal conductivity, making it highly efficient for thermoelectric applications. Its efficiency is measured by the dimensionless figure of merit (ZT), which is close to 1 at room temperature for optimized Bi₂Te₃-based materials. The layered crystal structure of Bi₂Te₃ reduces heat transport by phonons while allowing efficient movement of charge carriers, contributing to its superior thermoelectric performance.

Keywords: Thermoelectric Materials, Nanomaterials, Seebeck Effect, Electrical Conductivity.

Introduction

Thermoelectric materials are a unique class of materials that can directly convert thermal energy into electrical energy and electrical energy into cooling without the use of moving mechanical parts. Their performance depends on the relationship between electrical conductivity, thermal conductivity, and the Seebeck coefficient. Both n-type and p-type Bi₂Te₃ alloys are commonly used in thermoelectric modules for power generation and solid-state refrigeration. Typical applications include portable coolers, electronic device cooling, infrared detectors, and waste heat recovery systems.

Among the various thermoelectric materials investigated, bismuth telluride (Bi₂Te₃) has emerged as the benchmark material for room-temperature applications. It is a narrow-band-gap semiconductor with a layered rhombohedral crystal structure that promotes efficient charge transport while suppressing lattice thermal conductivity through enhanced phonon scattering. These characteristics result in a relatively high figure of merit, making Bi₂Te₃ highly suitable for thermoelectric cooling and power generation.

Bulk Bi₂Te₃ exhibits a maximum thermoelectric figure of merit (ZT) less than 1 at room temperature. Furthermore, the thermoelectric performance of Bi₂Te₃ can be significantly enhanced through alloying, doping, nanostructuring, and defect engineering, which optimize carrier concentration and reduce thermal conductivity. Consequently, Bi₂Te₃-based materials have found widespread applications in electronic cooling, infrared sensing, medical devices, portable refrigeration, and waste heat recovery. Owing to its exceptional room-temperature performance and technological importance, Bi₂Te₃ continues to be one of the most extensively studied thermoelectric materials in both academic research and industrial applications.

Several studies have demonstrated the potential of Bi₂Te₃-based materials for thermoelectric applications. E. Koukharenko *et al.* fabricated Bi₂Te₃ foils with thicknesses ranging from 10 to 60 μm using an ultrarapid quenching technique. Cicvarić K. *et al.* prepared Bi₂Te₃ thin films that exhibited a power factor of 88.2 μW m⁻¹ K⁻² at 520 K. Furthermore, Champness C. H. *et al.* prepared Bi₂Te₃-Sb₂Te₃ alloys and reported a maximum thermoelectric figure of merit of 1.5 at room temperature, demonstrating the significant performance enhancement achievable through alloy engineering.

. An Ag-doped room-temperature Bi₂Te₃-based thermoelectric material (BiSbTe₂Se) achieved excellent thermoelectric performance, with a maximum figure of merit (ZT) of 1.7 at 450 K and an average ZT of 1.5 between room temperature



Cover Page



and 575 K. The incorporation of Se atoms into the crystal structure optimized the entropy and enhanced lattice anharmonicity, reducing the thermal conductivity to an exceptionally low $0.4 \text{ W m}^{-1} \text{ K}^{-1}$. Meanwhile, Ag doping optimized the carrier concentration, preserving high electrical conductivity and significantly improving the power factor. As a result, a thermoelectric module fabricated from this material achieved a maximum conversion efficiency of 8% and an output power of 1.8 W under a 225 K temperature difference. Figure of merit of p-type $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$, after nanotexturing, researchers have achieved $zT = 1.4\text{--}1.8$, indicating excellent thermoelectric performance. Despite similar nanotexturing strategies, the reported zT values are only about 1.0–1.2 for n-type $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$ ($x < 1$). While p-type $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$ has reached $zT \approx 1.8$, the relatively lower $zT \approx 1.0\text{--}1.2$ of n-type $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$ has long limited the overall efficiency of Bi_2Te_3 -based thermoelectric devices. Due to complex relationship between carrier concentration and defect structure the enhancement in thermoelectric properties of n-type Bi_2Te_3 is more challengeable in comparison to p-type Bi_2Te_3 . Consequently, much recent research focuses on enhancing the performance of n-type Bi_2Te_3 -based alloys through defect engineering, band structure optimization, entropy engineering, and nanostructuring.

Zheng Ju et al. synthesized core-shell nano-structure of $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ with a seebeck coefficient of $145 \mu\text{V/K}$ at 500K. The electronic structure of bismuth telluride nanowires grown along the [110] and [015] crystallographic directions was investigated using the anisotropic effective-mass approach with the parabolic band approximation. Carrier confinement has a significant influence on the thermoelectric properties of bismuth telluride nanowires with cross-sectional dimensions below $30 \times 30 \text{ nm}^2$. Unlike excess-hole doping induced by impurities, quantum confinement simultaneously reduces the carrier concentration and lattice thermal conductivity while increasing the peak Seebeck coefficient. Moreover, the confinement effect is more pronounced for nanowires grown along the [015] crystallographic direction than for those oriented along [110], primarily due to the anisotropy in the effective carrier masses. For p-type nanowires, the maximum figure of merit was observed 2.8 at 480K for the dimension of $7 \times 7 \text{ nm}^2$. Moreover, the method of synthesis and sintering temperature also affect the thermoelectric properties of Bi_2Te_3 .

Theoretical studies on ultrathin Bi_2Te_3 have predicted a dramatic improvement in thermoelectric performance compared with the bulk material. By combining density functional theory calculations using VASP with quantum-mechanical structural optimization and the Landauer transport approach, researchers estimated that a single Bi_2Te_3 quintuple layer could achieve a room-temperature ZT of approximately 7.2, nearly an order of magnitude higher than that of bulk Bi_2Te_3 . This exceptional enhancement was primarily attributed to quantum confinement, which alters the electronic band structure and increases the density of transport modes near the valence band, thereby improving the thermoelectric efficiency.

Flexible electronics, which can withstand bending, rolling, folding, and stretching while maintaining their functionality, have attracted significant attention from both the scientific community and industry due to their potential for next-generation wearable devices, flexible sensors, displays, and energy-harvesting systems. Bi_2Te_3 -based flexible films are primarily fabricated using four main approaches: bulk thinning, physical or chemical deposition, paste casting, and template-assisted methods. Each technique offers distinct advantages in terms of film flexibility, thermoelectric performance, scalability, and compatibility with flexible substrates, making the choice of fabrication method dependent on the intended application. Flexible $\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ showed a figure of merit of 1.1 prepared from bulk thinning method.

Conclusion

Bismuth telluride remains one of the most efficient widely used thermoelectric materials for near room temperature applications and due to its excellent thermoelectric performance. Its high seebeck coefficient and good electrical conductivity contribute to a high thermoelectric figure of merit, making it suitable for both power generation and solid state cooling. Advances in nanostructuring, doping and composite fabrication have further enhanced its efficiency by optimizing charge transport while minimizing heat conduction. Despite challenges related to material cost, mechanical strength and long term stability, ongoing research continues to improve its performance and broaden its applications. Overall, the unique



Cover Page



thermoelectric properties of bismuth telluride make it a key material for sustainable energy conversion and environmentally friendly cooling technologies, with significant potential for future-efficient devices.

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