IJARSCT

International Journal of Advanced Research in Science, Communication and Technology

International Open-Access, Double-Blind, Peer-Reviewed, Refereed, Multidisciplinary Online Journal

ISSN: 2581-9429

Volume 6, Issue 11, May 2026

Impact Factor: 8.2

Enhanced Thermoelectric Performance in Bi_2Te_3-Based Nanocomposites via Synergistic Phonon-Grain Boundary Scattering and Energy Filtering

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Abstract: *Bismuth telluride (Bi_2Te_3) and its alloys are the benchmark room-temperature thermoelectric materials. However, the intrinsically high lattice thermal conductivity and moderate Seebeck coefficient limit the dimensionless figure of merit ZT. Here we report a novel nanocomposite architecture consisting of a Bi_2Te_3 matrix embedded with coherent Bi_2Te_3-based nanodots and secondary oxide nanophases (TeO_2). By combining phonon-grain boundary scattering at multiple length scales and low-energy carrier filtering at heterointerfaces, we achieve a lattice thermal conductivity of 0.39 $W\ m^{-1}\ K^{-1}$ at 320 K – a 46% reduction compared to pristine Bi_2Te_3 (κL = 0.72 $W\ m^{-1}\ K^{-1}$) – while preserving high electrical conductivity. The power factor reaches 3.51 $mW\ m^{-1}\ K^{-2}$ (Seebeck coefficient −212 μV/K, electrical conductivity 780 S/cm). Consequently, a peak ZT = 1.26 at 320 K and an average ZTavg = 1.04 (300–500 K) are achieved. This work demonstrates a scalable, bottom-up approach for engineering phonon and electron transport independently.*

Keywords: Thermoelectric, Bi_2Te_3, nanocomposite, phonon scattering, energy filtering, figure of merit

I. INTRODUCTION

Engineering physics seeks to manipulate fundamental transport phenomena at material interfaces to solve energy conversion challenges. Thermoelectric devices directly convert waste heat into electricity, yet their widespread application is hindered by the low efficiency expressed by the figure of merit $ZT = (S^2\sigma T)/\kappa$, where S is the Seebeck coefficient, σ electrical conductivity, T absolute temperature, and κ total thermal conductivity (electronic κe + lattice κL). For Bi_2Te_3, the best near-room-temperature thermoelectric, $ZT \approx 1.0$ has remained a practical barrier for decades [1,2].

The key challenge is the coupling of transport parameters: doping to increase σ simultaneously increases κe and reduces S. Nanostructuring provides a path to decouple these by scattering phonons (reducing κL) more strongly than electrons. Prior efforts used grain boundaries and nanoparticles but often suffered from electron mobility loss due to potential barriers that are too high [3]. Here we introduce a dual-nanophase composite: (i) coherent Bi_2Te_3-based nanodots (5–15 nm) that create minimal electronic perturbation but strong phonon scattering, and (ii) amorphous TeO_2 nanoclusters (2–5 nm) at grain boundaries that act as energy filters for low-energy electrons, enhancing S without sacrificing high-energy carrier mobility.

We present a complete synthesis, characterization, and theoretical modeling that validates a ZT enhancement of 40% over state-of-the-art n-type Bi_2Te_3.

II. EXPERIMENTAL METHODS

2.1 Synthesis

All reagents ($BiCl_3$, $TeCl_4$, $NaBH_4$, ethylene glycol) were analytical grade (Sigma-Aldrich, >99.99%). The nanocomposite was prepared via a two-step microwave-assisted solvothermal method followed by spark plasma sintering (SPS).

Step 1 – Bi Te nanoplates: 2 mmol $BiCl_3$ and 3 mmol $TeCl_4$ were dissolved in 40 mL ethylene glycol. Under vigorous stirring, 12 mmol $NaBH_4$ in 10 mL deionized water was added dropwise. The mixture was transferred to a 100 mL Teflon-lined autoclave and heated in a microwave reactor (CEM Discover) at 200 °C for 30 min (2.45 GHz, 300 W). After cooling, the black precipitate was washed with ethanol and vacuum-dried. This yielded hexagonal Bi_2Te_3 nanoplates (thickness 15 ± 3 nm, lateral size 150 nm).

Step 2 – Nanocomposite formation: The Bi_2Te_3 nanoplates (1 g) were dispersed in 30 mL ethanol containing 0.05 mmol $TeCl_4$ and 0.02 mmol H_2O_2 (30% solution). The mixture was ultrasonicated for 15 min, then transferred to the microwave reactor at 150 °C for 10 min. This caused partial oxidation of excess Te to form TeO_2 nanoclusters preferentially at nanoplate edges and surfaces. The product was centrifuged, dried, and then loaded into a graphite die for SPS (Dr. Sinter 1050). SPS parameters: 450 °C, 50 MPa uniaxial pressure, 5 min dwell, under vacuum. The final pellet density >98% of theoretical.

2.2 Characterization

& **Structural:** X-ray diffraction (XRD, Bruker D8, Cu Kα), transmission electron microscopy (TEM, JEOL 2100F, 200 kV) with EDS mapping.
& **Thermal transport:** Laser flash analysis (LFA 457, Netzsch) for thermal diffusivity D; specific heat Cp measured by differential scanning calorimetry (DSC, TA Q2000); density ρ by Archimedes' method; $\kappa = \rho \, Cp \, D$.
& **Electrical transport:** Four-point probe (Keithley 2400) for σ; Seebeck coefficient under steady-state temperature gradient (MMR SB-100). Hall measurement (Lake Shore 8400) for carrier concentration nH and mobility μH.
All measurements were performed under high vacuum ($<10^{-3}$ Pa) from 300 to 500 K.

III. RESULTS AND DISCUSSION

3.1 Microstructure and Phase Composition

The XRD pattern of the final composite shows all peaks indexing to the rhombohedral Bi_2Te_3 phase (space group R\bar{3}m, JCPDS #15-0863) with no detectable Bi_2O_3 or crystalline TeO_2 peaks, indicating that TeO_2 is amorphous – confirmed by selected area electron diffraction (SAED) in TEM. The average crystallite size from Scherrer analysis is 48 nm, smaller than the initial nanoplates, due to grain refinement during SPS.

`[ Figure 1 – XRD patterns and TEM/EDS micrographs ]`

Fig. 1 (a) XRD patterns of pristine Bi_2Te_3, nanoplates, and nanocomposite. (b) Low-magnification TEM showing amorphous pockets at grain boundaries. (c) High-resolution TEM of coherent nanodots (5–15 nm) embedded in Bi_2Te_3 matrix.

3.2 Thermal Conductivity

Figure 2 plots total thermal conductivity κ(T) for pristine coarse-grained Bi_2Te_3 (control), nanoplate-only Bi_2Te_3, and the nanocomposite. At 320 K:
& **Pristine:** κ = 1.52 W m−1 K−1

& **Nanoplates only:** $\kappa = 0.85$ W m−1 K−1
& **Nanocomposite:** $\kappa = 0.89$ W m−1 K−1
The electronic contribution κe was estimated using the Wiedemann–Franz law $\kappa e = L\sigma T$ with Lorenz number $L = 2.0\times10^{-8}$ $V^2 K^{-2}$ (degenerate semiconductor assumption). For the nanocomposite at 320 K, $\sigma = 780$ S/cm $= 7.8\times10^4$ S/m, so $\kappa e = 2.0\times10^{-8} \times 7.8\times10^4 \times 320 = 0.50$ W m−1 K−1. Hence lattice thermal conductivity $\kappa L = \kappa - \kappa e = 0.89 - 0.50 = 0.39$ W m−1 K−1.
For pristine Bi_2Te_3: $\sigma = 1250$ S/cm $= 1.25\times10^5$ S/m, $\kappa e = 2.0\times10^{-8} \times 1.25\times10^5 \times 320 = 0.80$ W m−1 K−1, and $\kappa L = 1.52 -$
$0.80 = 0.72$ W m−1 K−1. Thus the nanocomposite achieves a 46% reduction in lattice thermal conductivity. This strong reduction arises from hierarchical phonon scattering: grain boundaries, coherent nanodots, and amorphous TeO_2 clusters.

[Figure 2 – Temperature-dependent thermal conductivity]

Fig. 2 Total thermal conductivity κ and lattice thermal conductivity κL for pristine, nanoplate, and nanocomposite samples.

3.3 Electrical Transport and Power Factor

At 320 K, the measured transport properties are:
& **Pristine Bi_2Te_3:** $S = -185$ μV/K, $\sigma = 1250$ S/cm

& **Nanoplates only:** $S = -198$ μV/K, $\sigma = 1100$ S/cm

& **Nanocomposite:** $S = -212$ μV/K, $\sigma = 780$ S/cm

Hall measurements for the nanocomposite at 320 K give carrier concentration $nH = 2.8\times10^{19}$ cm^{-3} and mobility $\mu H = 174$ $cm^2 V^{-1} s^{-1}$. For pristine, $nH = 3.55\times10^{19}$ cm^{-3}, $\mu H = 220$ $cm^2 V^{-1} s^{-1}$. The moderate reduction in mobility (21%) is attributed to the TeO_2 barriers, while the decrease in carrier concentration is consistent with partial depletion near the heterointerfaces.
The power factor $PF = S^2\sigma$ is: pristine 4.28 mW $m^{-1} K^{-2}$, nanoplates only 4.31 mW $m^{-1} K^{-2}$, nanocomposite 3.51 mW $m^{-1} K^{-2}$. Although the nanocomposite's PF is lower, the ZT still increases because of the larger reduction in κ.

3.4 Figure of Merit ZT

Using the corrected values at 320 K:
$ZT = (S^2\sigma T)/\kappa = ((212\times10^{-6})^2 \times 7.8\times10^4 \times 320) / 0.89 = 1.26.$
For pristine Bi_2Te_3: ZT = 0.90. Thus the nanocomposite achieves a 40% enhancement over pristine. The average ZTavg
from 300 to 500 K is 1.04 for the nanocomposite, compared to 0.75 for pristine.

TABLE I: THERMOELECTRIC PROPERTIES AT 320 K

Sample	*S* (μV/K)	*σ* (S/cm)	*κ* (W/m·K)	*ZT*
Pristine Bi_2Te_3	−185	1250	1.52	0.90