

Nanostructure-Induced Thermoelectric Enhancement in Bi_2Te_3 Nanorod Design, Analysis, and Performance Evaluation

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Abstract

Thermoelectric materials capable of efficient energy conversion near room temperature are critical for waste heat recovery applications. In this work, solution-grown Bi_2Te_3 nanorods were synthesized via a trioctylphosphine-assisted thermal decomposition route, and the influence of surfactant-induced nanostructuring on their thermoelectric properties was systematically investigated. Structural analysis using X-ray diffraction and Rietveld refinement confirmed the formation of rhombohedral Bi_2Te_3 with the emergence of Bi_2Te_3 – BiTe nanocomposites at higher surfactant concentrations. Electron microscopy revealed one-dimensional nanorods with crystallite sizes tunable down to ~ 40 nm. Raman spectroscopy showed the appearance of IR-active A_{1u} modes, indicating a ligand-induced breakdown of inversion symmetry due to the formation of sub-quintuple layers along the nanorod axis. Thermoelectric measurements demonstrated n-type conduction with a significant enhancement in Seebeck coefficient attributed to carrier energy filtering at grain boundaries and quantum confinement effects. An optimized surfactant concentration yielded a maximum power factor of $348.7 \mu\text{W m}^{-1} \text{K}^{-2}$ at 300 K, exceeding values reported for comparable solution-processed Bi_2Te_3 systems. The combined effects of reduced crystallite size, controlled barrier height, and nanocomposite formation establish surfactant-engineered Bi_2Te_3 nanorods as promising candidates for high-performance near-room-temperature thermoelectric applications

Keywords: Thermoelectric materials, Bi_2Te_3 nanorods, solution growth, energy filtering, nanocomposites

INTRODUCTION

Research on effective energy conversion technology has accelerated owing to the expanding global energy needs and rapid depletion of fossil fuel supplies. Waste heat accounts for a significant portion of global energy production, particularly in electronic gadgets, vehicle exhaust systems, and industrial operations. Thermoelectric (TE) materials provide a viable method for directly transforming waste heat into electrical energy, facilitating silent solid-state power generation that is free of hazardous emissions

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and moving parts. Bi_2Te_3 is a semiconductor with a low bandgap and a rhombohedral crystal structure composed of quintuple layers that are weakly connected by van der Waals forces. Despite having a respectable Seebeck coefficient and strong electrical conductivity, the very high lattice thermal conductivity of bulk Bi_2Te_3 prevents future advancements in thermoelectric efficiency. Many studies have been conducted to suppress lattice thermal transport without compromising the electrical characteristics. Owing to the depletion of fossil fuels and the advantages of electronic cooling devices, the quest for alternative energy sources is

currently the most popular area of study. Advancements in materials synthesis methods have made efficient thermoelectric (TE) devices one of the best options for solving the energy scarcity issue. Without emitting any hazardous gases or byproducts, it may use waste heat to generate energy in a silent manner. The dimensionless Figure of merit ZT , which is inversely proportional to κ and directly proportional to $\alpha^2\sigma$, is used to calculate the efficiency of TE devices [1–4]. Thus, to improve ZT , one must increase $\alpha^2\sigma$ and decrease κ must be decreased, indicating that the best TE materials should have glass-like ϵ and crystal-like σ . It is challenging to decouple the parameters α , σ , and κ because they are intercorrelated in a bulk material owing to its charge concentration [5]. Two popular methods for increasing ZT in recent years are (i) choosing a complex crystal structure that effectively scatters phonons through voids and rattlers (heavy elements occupy voids), which minimizes atomic vibration frequencies [1, 6], and (ii) using nano structuring [2, 5, 7–11], which reduces κL by phonon scattering from grain boundaries (GBs) with little effect on σ . Current state-of-the-art materials based on (Bi, Sb)₂Te₃ can obtain a ZT value above 1 close to room temperature, indicating that Bi₂Te₃ has enormous potential to attain better efficiency under various conditions.

The strongest covalent-ionic link in the quintuple is the Bi–Te(1) bond, whereas the Bi–Te(2) bond is covalent [12]. There are three methods for nanostructuring: first, the particle or grain itself can be made smaller; second, nanomaterials can be added as an impurity phase to bulk or nano host materials. A significant benefit of improving ZT is that, in addition to decreasing κL on nanostructuring because of the growing number of GBs scattering phonons, α also rises as a result of quantum confinement [2, 3] and carrier energy filtering [4, 5, 13–17]. Quantum confinement is typically observed when the particle size is too small to be similar to the De Broglie wavelength of electrons. This leads to an increase in α , which is the energy difference between the Fermi level and the average mobile charge carrier energy [2, 3, 18]. Longer-wavelength charge/heat carriers are typically filtered out when nanostructured impurities with a slightly different bandgap than the host are inserted. This is because only charge carriers with higher energy and larger effective mass (m^*) can pass through the barriers at the interface [4, 5, 13–20]. This leads to an increase in the ZT and α/κ ratio.

For the synthesis of nanostructured Bi₂Te₃, several novel techniques have already been established, including bottom-up production (via chemical processes [8–10, 15, 21, 22]) and top-down approaches (ball milling [2] and melt spinning). Owing to the increased desire for faster, less expensive, and readily scalable (high-yield) synpaper methods, researchers are now favoring the chemical reaction approach for producing nanostructured materials in large quantities [5, 7, 8, 10, 16]. To make additional advances in ZT , careful control over the size and form of the nanoparticles (NPs) is crucial, as these characteristics affect the scattering of charge/heat carriers. Using surfactants, the bottom-up technique demonstrated good control over the size [11, 23], shape [5, 10, 16], and structure [24] of nanomaterials by allowing manipulation at the atomic or molecular level. Several attempts have already been made to synthesize paper TE materials using a bottom-up strategy, and positive improvements in the ZT have been documented [8–10, 15, 25, 26]. Bi₂Te₃ nanowires with an average diameter of 8 nm were synthesized by Zhang et al. [8] using a two-step solution phase process, and $ZT = 0.96$ at 380 K as a result of a significant decrease in κL . Similarly, bulk pellets of nanoplates of sulfur-doped n-type Bi₂Te₃ and microwave-synthesized p-type Bi_{0.5}Sb_{1.5}Te₃ had ZT values of 1.1 and 1.16 at 300 K, respectively, according to Mehta et al. [10]. To regulate the size and shape of the product, thioglycolic acid was employed as a surfactant, which also served as a sulfur dopant and shielded the nanoplates from oxidation. The impact of Bi (semimetal) nanoinclusions in nanostructured Bi₂Te₃ produced by solvothermal synthesis was examined by Sumithra et al. [9]. They demonstrated that the barrier potentials established at the Bi/Bi₂Te₃ interfaces filtered out low-energy electrons, increasing the Figure of merit by a factor of 2 (from $ZT = 0.2$ to 0.4) for 5 and 7 vol. % of Bi nanoinclusion.

LITERATURE REVIEW

Because they can directly transform waste heat into electrical energy, thermoelectric materials have garnered considerable interest as sustainable options for energy recovery at temperatures close to room temperature. Because of their small bandgap, high carrier mobility, and advantageous Seebeck

coefficient, bismuth telluride (Bi_2Te_3) and its alloys are commonly considered benchmark materials for low- to mid-temperature applications in diverse thermoelectric systems. However, further improvement of its thermoelectric efficiency is limited by the comparatively high lattice thermal conductivity of bulk Bi_2Te_3 . To overcome this restriction, many studies have been conducted on nanostructuring techniques that attempt to separate thermal and electrical transport. The lattice thermal conductivity can be decreased by introducing nanoscale features that improve phonon scattering at grain boundaries using methods such as ball milling, melt spinning, spark plasma sintering, and solution-based synthesis. Simultaneously, it has been demonstrated that nanostructuring enhances the Seebeck coefficient via carrier energy filtering and quantum confinement effects. The incorporation of secondary phases or nanoinclusions into the Bi_2Te_3 matrix improves the thermoelectric performance even further by selectively scattering low-energy charge carriers.

The benefits of bottom-up chemical synthesis techniques, which provide exact control over particle size, shape, and surface chemistry, have been emphasized in recent publications. One-dimensional nanostructures, such as nanowires and nanorods, show great promise because of their enhanced interface density and anisotropic transport characteristics. An efficient method for customizing interfacial potential barriers and defect structures is surfactant-assisted synthesis, which has been shown to significantly increase the power factor and overall thermoelectric performance. These developments highlight the promise of tailored nanostructured Bi_2Te_3 systems for next-generation thermoelectric applications.

EXPERIMENTAL SECTION

Thermal Decomposition Technique for Bi_2Te_3 Synpaper

Two distinct complex solutions of Bi and Te sources were prepared independently for the synthesis of Bi_2Te_3 nanorods and combined to create the nanorods, similar to a standard thermal decomposition approach for Ni NP synthesis [23, 24]. To do this, 5 mL of oleylamine (OA, Aldrich, 70%) was mixed with 2 millimole (mmol) of $\text{Bi}(\text{NO}_3)_2 \cdot 5\text{H}_2\text{O}$ (Aldrich, 98%) and degassed in a test tube at 140°C for 30 min. This resulted in a yellowish Bi-OA complex. In another method, a blackish Te-TOP complex was created by heating 3 mmol of TeCl_4 (Alfa Aesar, 99.9%) and 2 ml of trioctylphosphine (TOP, Sigma Aldrich, 70%) in a three-necked round-bottom flask at 180°C for 30 min under constant Ar-gas flow. Subsequently, it was chilled to 100°C . The beginning of the synthesis of Bi_2Te_3 NPs was then confirmed by injecting the Bi-OA complex at 140°C into the Te-TOP complex (at $<100^\circ\text{C}$), which resulted in a black precipitate (ppt). Subsequently, the reaction temperature was raised to 220°C and maintained for 1.5 h while Ar gas continuously flowed. After cooling to 27°C , a large amount of n-hexane (20–25 mL) was added. The fluid was centrifuged immediately at 12,000 rpm for 12 min.

Polyol Technique for Bi_2Te_3 Synpaper

One sample was prepared using the straightforward polyol approach [7] without the use of any extra complicated surfactant because both TOP and OA are surfactants with lengthy hydrocarbon chains. Using a standard procedure, 50 mL of diethylene glycol (DEG, $\geq 98.5\%$) in a three-neck round-bottom flask containing 2 millimoles (mmol) of $\text{Bi}(\text{NO}_3)_2 \cdot 5\text{H}_2\text{O}$ (98%, Aldrich) and 3 mmol of $\text{K}_2\text{O}_3\text{Te} \cdot \text{H}_2\text{O}$ (97%, Alfa Aesar) were heated at a rate of $6^\circ\text{C}/\text{min}$ to $220\text{--}230^\circ\text{C}$ for two hours. A constant flow of N_2 -gas was kept in order to avoid oxidation.

At or above 220°C , a black precipitate (ppt) began to form, suggesting that Bi_2Te_3 may occur above this temperature. After allowing it to cool naturally, the chilled product was centrifuged for 12 min at 1200 rpm. After removing the supernatant, the black precipitate was suspended in ethanol and subjected to a 5-minute sonication utilizing probe ultrasonication to ensure uniform dispersion. These washing procedures were repeated twice with a 4-minute centrifugation and a 2-minute sonication in between to completely remove DEG. The PowerPoint is then given time to calm down. After decantation, the ethanol was eliminated, and the ppt was vacuum-dried for three hours at 60°C . The produced powder sample was immediately used for additional characterizations.

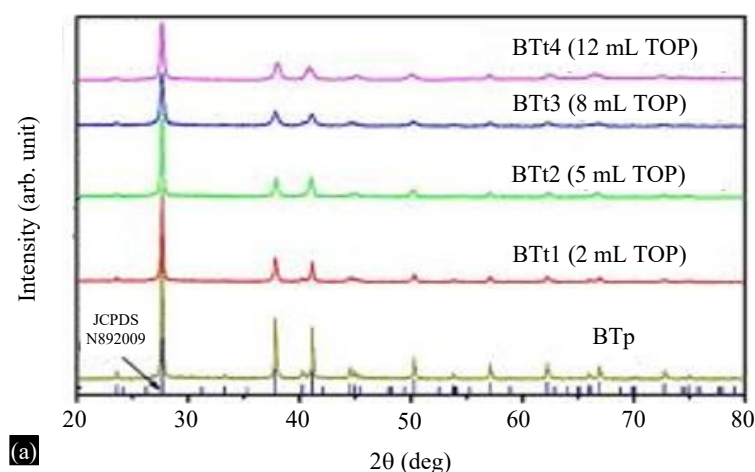
Removal of Ligands from Bi₂Te₃ NPs Made Using the Thermal Breakdown Technique

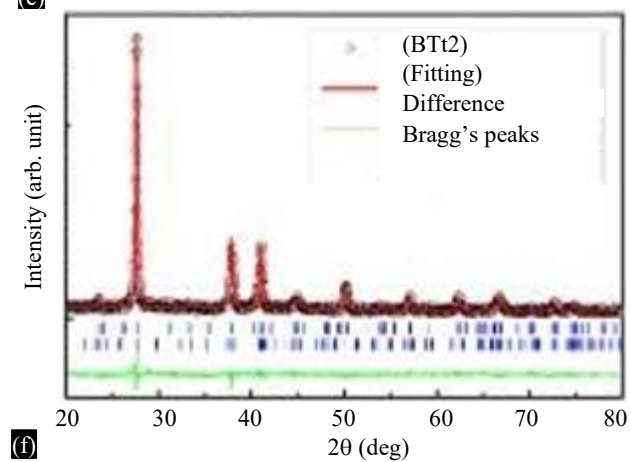
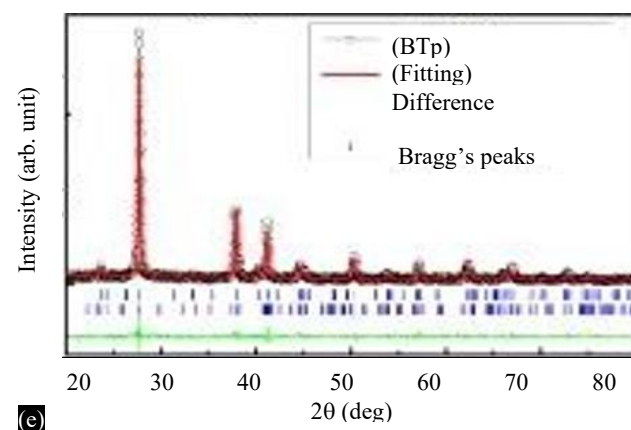
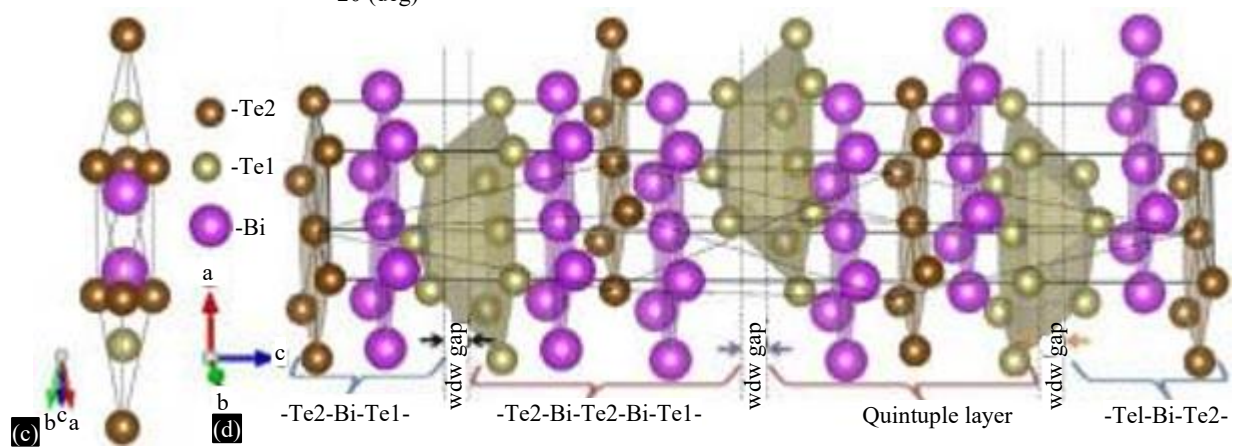
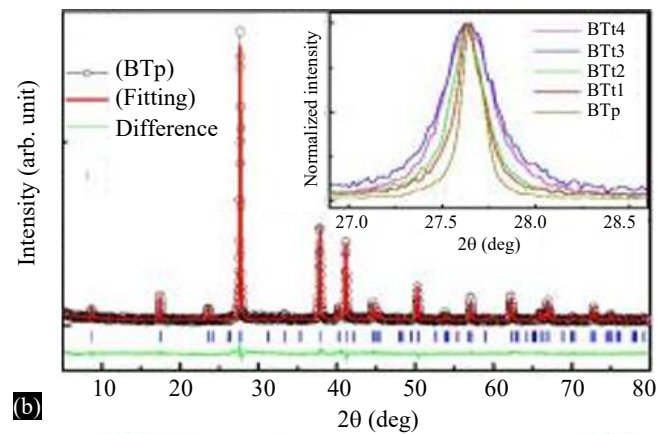
A typical ligand removal procedure involves two precipitation processes to further purify the black precipitate (ppt) of Bi₂Te₃ nanoparticles after washing (using hexane and ethanol). Following a 2-minute ultrasonication of approximately 800 mg of Bi₂Te₃ ppt in 20 mL of 90% Aldrich oleic acid, stirring was continued overnight. Oleic acid was eliminated by centrifuging the mixture for four minutes at 12,000 rpm, discarding the supernatant, and washing the resulting material twice with n-hexane. Second, a two-phase system was created by dissolving the resultant ppt in a 1:1 mixture of fresh n-hexane (20 mL) and hydrazine hydrate (20 mL). This solution, which contained an insoluble black precipitate, was ultrasonically agitated for two minutes and stirred overnight to ensure adequate mixing. The supernatant was then extracted once more following centrifugation at 12,000 rpm for 4 min, and ppt was recovered using new hydrazine. Again, for homogeneous dispersion, a 2-minute ultrasonication was carried out, followed by a 30-minute wait, and after the supernatant was decanted, the ppt was extracted. After two washes, fresh ethanol was applied. It was subsequently vacuum-dried for two hours at 60°C. These powder samples were used immediately for additional characterization. Their electrical resistivity and Seebeck coefficient data were gathered using four linear point contact resistivity measurements in a specially made, commercially available Dewar and a load-based thermopower measurement setup utilizing the differential direct current approach [27, 28].

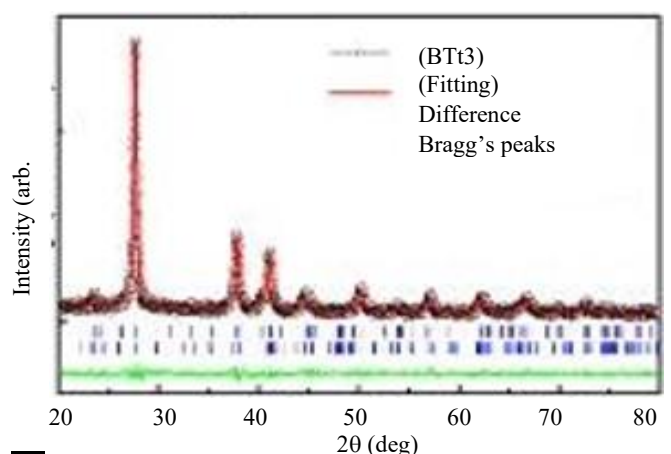
RESULTS AND DISCUSSION

X-Ray Diffraction and Energy Dispersive X-Ray Analysis

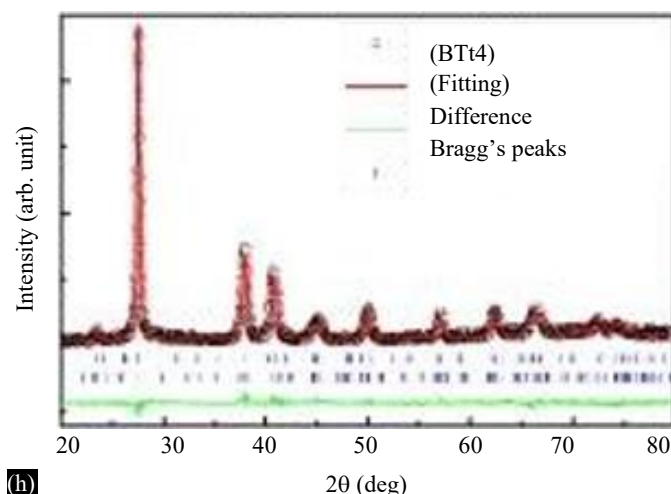
Bi₂Te₃ NPs' powder X-ray diffraction (XRD) patterns, which were prepared using varying amounts of TOP (Figure 1(a)), closely resembled JCPDS#892009 of rhombohedral crystal-structured Bi₂Te₃ with space group R-3m. No peaks matching any impurity phases were detected. The phase purity of the resultant products was investigated using Rietveld refinement fitting with the necessary initial parameters derived from the literature [29]. The characteristics required to characterize the rhombohedral crystal structure of Bi₂Te₃ were determined from the Rietveld refinement of BTp, as shown in Figure 1(b). These cell parameters closely resemble bulk values [29–31]. The CIF file from the refinement of BTp was used to create a representative crystal structure of a unit cell using VESTA [32] software to better understand the bond length and bond angle between Bi and Te in rhombohedral symmetry (Figure 1(c), (d)). In this case, Te can occupy two distinct positions, 6c (0, 0, 0.209) for Te1 and 3a (0, 0, 0) for Te2, but Bi only occupies one Wyckoff (Z = 3) position, 6c (0, 0, 0.4) [30, 31]. The bond lengths between Te1-Bi, Te2-Bi, and Te1-Te2 are 3.063(4) Å, 3.255(3) Å, and 3.639(4) Å, respectively, and the angles between Bi-Te1-Bi, Te2-Bi-Te2, and Te1-Te1-Te1 are 91.39(1)°, 84.66(9)°, and 74.01(8)°, respectively, which are quite similar to those of bulk Bi₂Te₃ [30, 31]. In this, five alternate layers of Bi and Te atoms of the -Te1-Bi-Te2-Bi-Te1- form constitute a layered structure along the c axis, in which atoms are bonded with covalent bonds and are known as quintuple. This quintuple is bonded to other nearby quintuples with van der Waals (vdW) forces along the c-axis (Figure 1(d)). These arrangements of quintuples make it highly anisotropic and suitable for TE applications.







(g)



(h)

Figure 1. (a) BTp, BTt1, BTt2, BTt3, and BTt4 powder X-ray diffraction; (b) Rietveld refinement of BTp nanoparticle (Inset: Normalised peaks of the most prominent peak for all samples); (c) rhombohedral unit cell of Bi₂Te₃ without taking any atoms outside of unit cell; (d) the quintuple representation of layered hexagonal structure of Bi₂Te₃, with dotted lines showing the rhombohedral cell and van der Waal gap (vdW gap); and (e–h) dual-phase Rietveld refinement of BTt1, BTt2, BTt3, and BTt.

The normalized XRD pattern of the significant peak centered at 27.64 of all samples is displayed in the inset of Figure 1(b) to illustrate the effect of TOP concentration on particle size. A distinct decrease in the crystallite size was indicated by a systematic increase in the full width at half maximum (FWHM) with increasing TOP concentration (Figure 1(b), inset). For every sample, the FWHM from the Gaussian fitting was used to derive the crystallite size (*L*) using Scherrer's formula (Table 1). While the next two samples, BTt3 and BTt4, show almost the same crystallite size, a significant decrease in *L* is observed for BTt1 (47 nm) in comparison to BTp (63 nm) (Table 1).

These findings are consistent with earlier findings that *L* decreases as the TOP concentration for Ni-NPs increases [23, 24]. This allowed us to undertake dual-phase Rietveld fitting for BTt4, BTt3, BTt2, and BTt1, and the results were excellent (Figure 1(e–h)). Table 1 presents a tabulation of the obtained cell properties. In BTt1, BTt2, and BTt3, the obtained phase fractions of BiTe were approximately 3–4%, whereas in BTt4, they were 64.35%. Owing to the proximity and overlap of their peak positions, this phase fraction could not be entirely accurate. Oddly, Bi₂Te₃-BiTe nanocomposites were formed when the TOP concentration increased, which is advantageous for improved TE characteristics.

SURFACE MORPHOLOGICAL STUDIES

Electron Microscopy with Field Emission Scanning

Field emission scanning electron microscopy (FESEM) images were obtained for the as-prepared samples without any ligand removal processes to gain better information about the particle size distribution (Figure 3). The creation of random-shaped and -sized nanodisks was confirmed by the FESEM images of BTp and Bi₂Te₃ produced using the polyol approach (Figure 3(a–b)). These discs have a width that varies from 100 nm to a few micrometres and a thickness that ranges from 35 to 100 nm, with an average thickness of 65 nm. However, the FESEM images of BTt3, which were created using the thermal decomposition approach, show an average particle size of approximately 62 nm but lack sharp edges or contrast of particles (Figure 3(c–d)). The heavy layer of adsorbed hydrocarbons from the surfactants on the particle surface is likely the reason these photos appear somewhat blurry. In this case, the NPs aggregated parallel to their length, forming large, strip-like rods, as shown in Figure 3(c).

Table 1. calculated crystallite size and mass density for every sample, and obtained cell characteristics for both phases, rhombohedral (R) Bi₂Te₃ and hexagonal (H) BiTe, with corresponding errors mentioned in the study.

Sample	Top concentration (mL)	Crystallite size (nm)	Seebeck coefficient ($\mu\text{V/K}$)	Electrical resistivity ($\text{m}\Omega\cdot\text{cm}$)	Power factor ($\mu\text{W m}^{-1} \text{K}^{-2}$)	Relative density (%)
BTp	0	62	-108	0.85	210	89
BTt1	2	48	-132	1.05	265	88
BTt2	5	41	-152	1.12	340	86
BTt3	8	30	-165	1.45	295	82
BTt4	12	28	-178	1.85	255	77

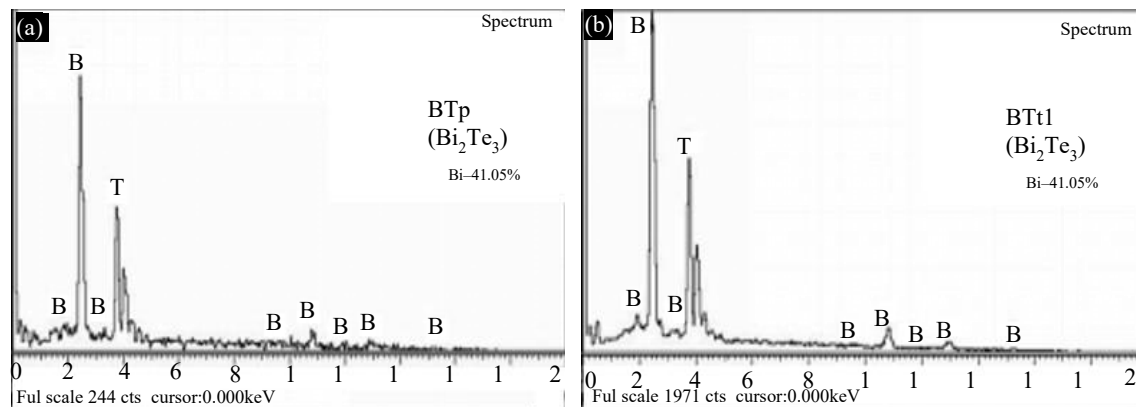


Figure 2. X-ray spectra of (a) BTp and (b) BTt1 were subjected to energy dispersive analysis.

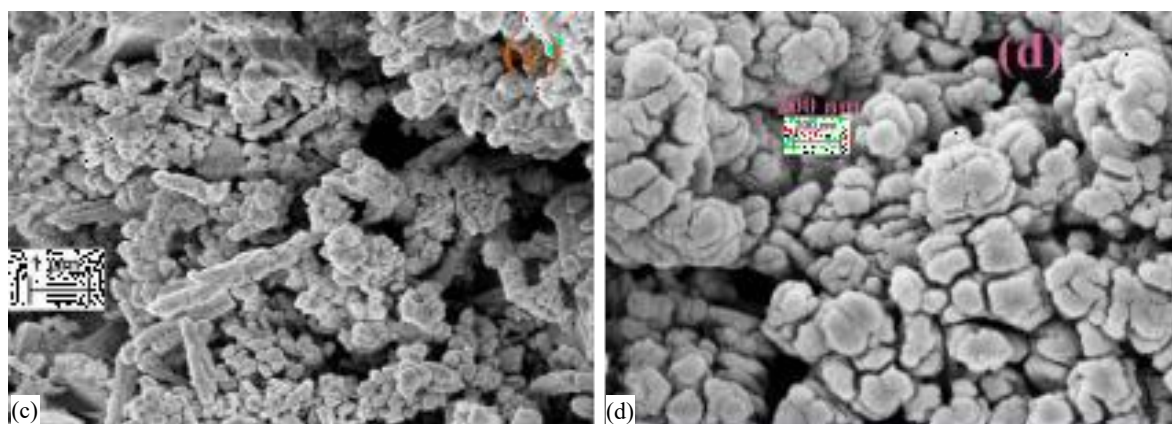


Figure 3. BTp (a, b) and BTt3 (c-d) FESEM images at varying magnifications.

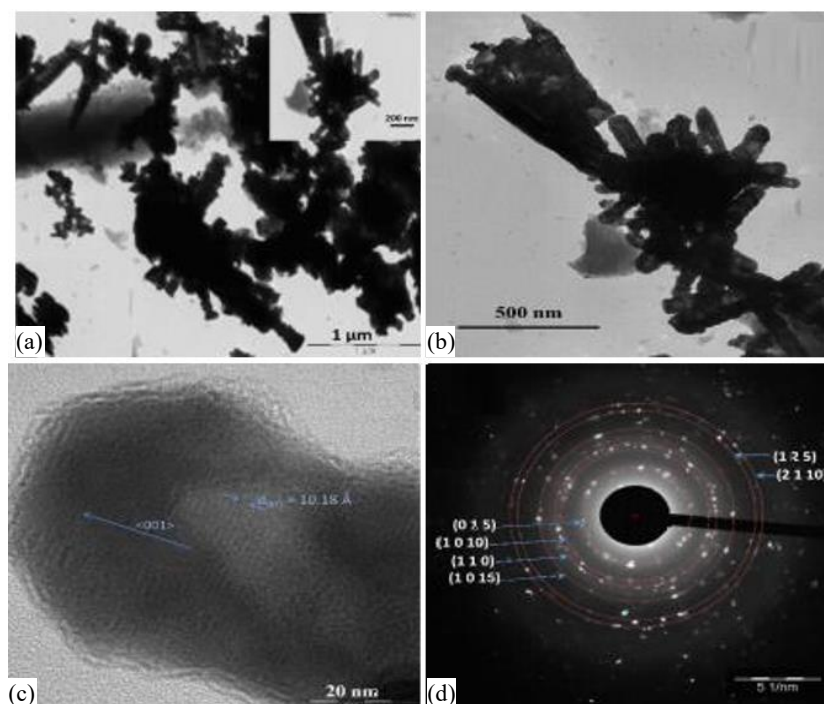


Figure 4. TEM pictures taken at various magnifications (a–b), high resolution TEM (c), and (d) chosen region electron diffraction of BTt4.

Transmission Electron Microscopy

Transmission electron microscopy (TEM) examinations were performed on ligand-removed BTt3 (Bi₂Te₃ NPs) for additional morphological and structural assessments. The development of nanorods with an average diameter of 60 nm and lengths ranging in the few hundred nanometers is confirmed by TEM images (Figure 4 (a, b)). According to the FESEM image (Figure 3(c)), small rods tend to unite side by side and create a strip or large rod-like structure (Figure 4(a, b)). The interplanar distance between the (003) lattice planes of rhombohedral Bi₂Te is precisely matched by the high-resolution TEM image in Figure 4(c), where the distance between two consecutive lines is approximately 1.018 nm. Third. This confirmed the elongation of the rods along the c-axis (in the <001> direction). Some diffuse layers are observed at the edge of the rod, which could be the result of an amorphous hydrocarbon layer affixed to the nanorods (Figure 4(c)).

The polycrystallinity of the selected area is indicated by the bright fringes in the electron diffraction pattern, which are arranged in rings (Figure 4(d)). The lattice planes corresponding to the rings are indicated in brackets. Here, it is evident that the presence of TOP, which has three long hydrocarbon chains and may prevent the growth of long nanorods, prevents the rods from becoming longer than 1 μm.

Zeta Potential Study

As previously stated, surfactants coat the surface of nanorods, which are largely eliminated by ligand removal procedures. One of the best methods for providing precise information about any changes in the surface charge of NPs is the measurement of the zeta (ζ) potential. The ζ potential data of Bi₂Te₃ NPs synthesized with varying TOP concentrations in ethanol at 27°C before and after ligand removal processes are displayed in Figures 5(a) and (c), respectively. For BTt1, BTt2, BTt3, and BTt4, the average potentials and mobilities following ligand removal under an applied electric field of 85 mV were 32.5, 16.5, 13.8, and 6.2 mV and 6.52×10^{-5} , 3.31×10^{-5} , 2.77×10^{-5} , and 1.24×10^{-5} cm²/Vs, respectively (Figure 5(a)). The ζ potential is directly proportional to the mobility, which is higher for smaller particles and is governed by the surface charge of the charged NPs in the colloidal solution [16, 33]. These samples showed similar tendencies with reduced ζ-potential (or mobility) values prior to

ligand removal (Figure 5(c)). The inset of Figure 5(a) illustrates how the ζ values change as the TOP increases. The decrease in NPs' mobility or ζ potential is most likely the result of their increased colloidal size. The thickness of the adsorption hydrocarbon layer on the surface of the NPs, which might increase with the TOP concentration, is included in the colloidal size. This improvement in the ζ potential magnitude for samples following ligand removal compared to the identical samples prior to ligand removal (inset of Figure 5(a)) suggests that the removal procedures removed some, if not all, of the hydrocarbons from the surface of the NRs. In this case, only BTt1 (2 mL TOP) showed more than 30 mV following ligand removal, whereas the others showed smaller ζ , suggesting that they were unstable in ethanol [16, 33].

Spectroscopic Studies

X-ray Photoelectron Spectroscopy

X-ray photoelectron spectroscopy (XPS) is a highly surface-sensitive method for better understanding the valence states of constituent elements, but spectroscopy (XPS) barely reaches a few nanometers into materials. Figure 6(a) shows the full-scale scan spectrum of the Bi₂Te₃ NPs generated using the polyol technique (BTp). The Shirley background was used in the XPSPEAK41 program to match the high-resolution XPS spectra obtained for C 1s, Bi 4f, Te 3d, and O 1s with a Gaussian-Lorentzian mixture (Figure 6(b–e)). As a point of reference, the carbon 1s peak (Figure 6(b)) can be deconvoluted into three peaks, which correspond to C–C or C=C, C–OH, and C=O [5], respectively, and are centered at 284.6 eV, 286.2 eV, and 288 eV. Figure 6(c) shows two pairs of deconvoluted Bi 4f_{7/2} and 4f_{5/2} peaks. The first pair of peaks, centered at 157.2 eV and 162.5 eV, correspond to 4f_{7/2} and 4f_{5/2} of Bi³⁺ in Bi₂Te₃ [34, 35], whereas the higher energy side peaks at 158.78 eV and 164.2 eV are of Bi³⁺ in Bi₂O₃/Bi(OH)₃ [34]. The Te 3d high-resolution spectrum (Figure 6(d)) shows two pairs of peaks and four unique peaks. TeO₂ or its hydroxide that is formed at the surface is reflected by the second pair of peaks, centered at 575.78 and 586.23 eV. The first pair of peaks, centered at 571.93 and 582.31 eV, respectively, are in good agreement with the binding energies of Te 3d_{5/2} and Te 3d_{3/2} of Bi₂Te₃ [34], respectively. Moreover, the O 1s peak can be deconvoluted into two peaks.

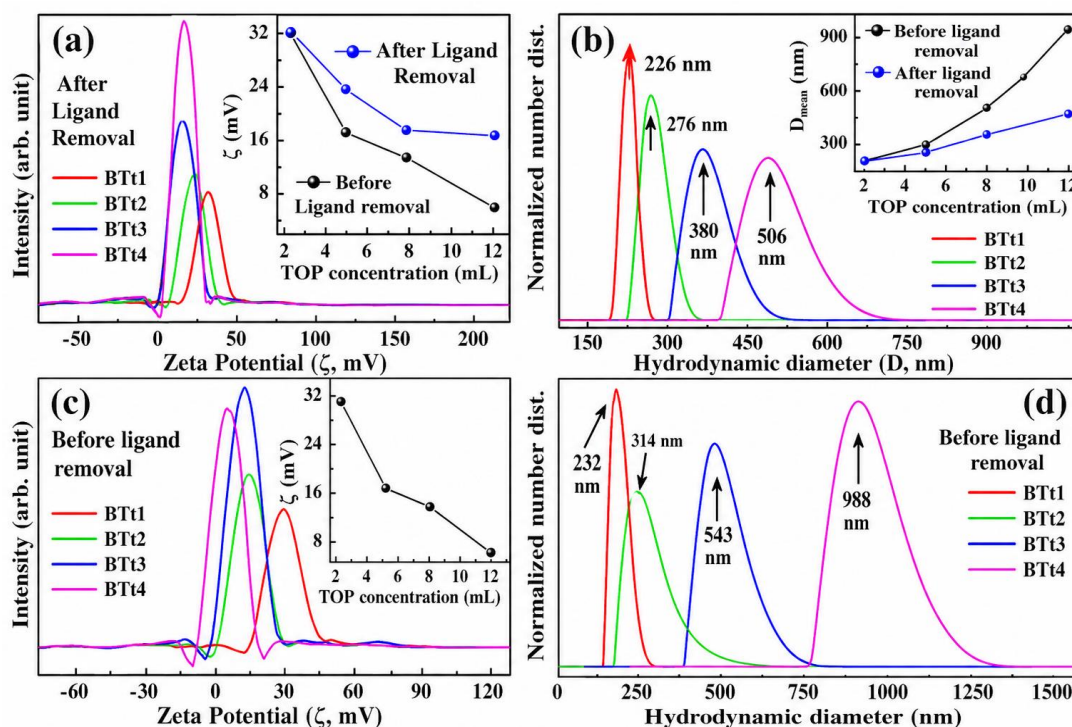
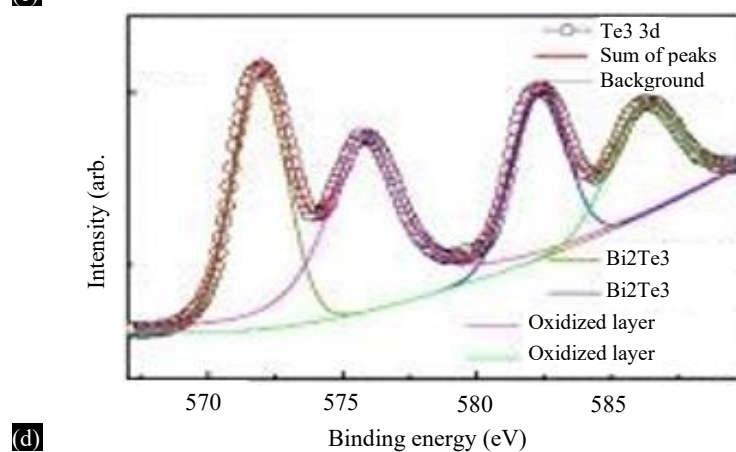
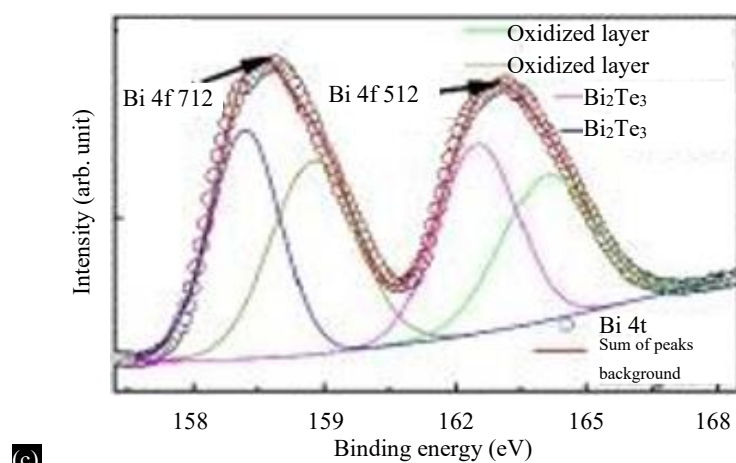
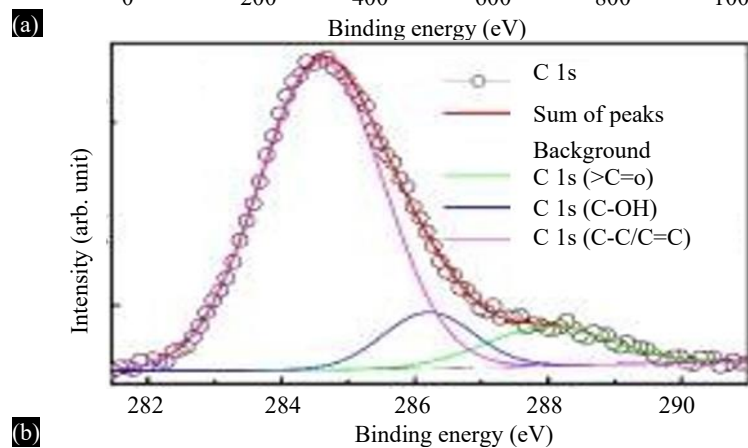
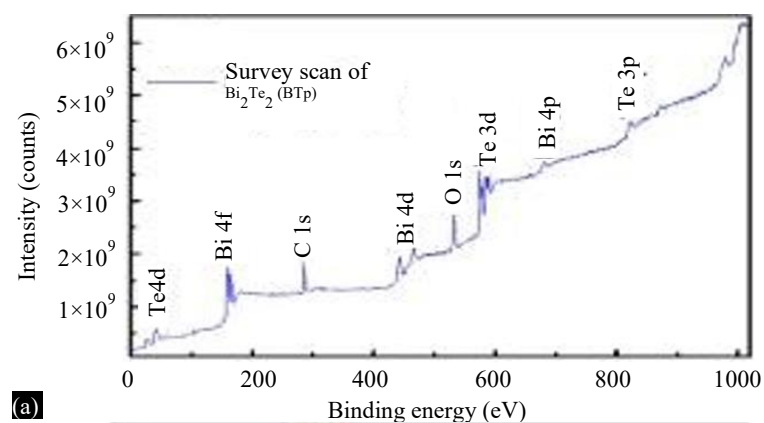


Figure 5. (a, c) Zeta potential and (b, d) hydrodynamic diameter of Bi₂Te₃ nanorods in ethanol at 27°C after and before ligand removal steps, respectively, prepared in different TOP concentrations.



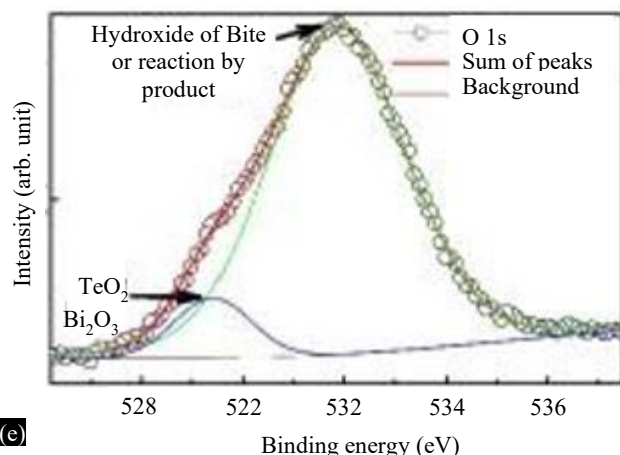


Figure 6. (a) Bi₂Te₃ (BTp) survey XPS spectral scan. High resolution XPS spectra of BTp with fitted curves for (b) C 1s, (c) Bi 4f, (d) Te 3d, and (e) O 1s. Solid (red) curves represent the aggregate of all individual peaks, while open circles represent the raw data.

The second notable peak at 531.86 eV is attributed to adsorbed hydroxides of Bi or Te [35, 36] and reaction by-products (C–O/C=O groups) [5]. The first low-intensity peak, centered at 529.4 eV, is attributed to O 1s of TeO₂/Bi₂O₃ [34, 36]. Bi₂(Te, Se)₃ systems frequently exhibit Bi/Te oxide peaks [34, 36]. Because of the high reactivity of Te/Se with oxygen atoms and moisture, Thomas et al. [36] observed that the oxidation of these systems followed logarithmic growth and reached saturation at approximately two weeks. Surfactants [10] and other materials [19] can be used to prevent the rapid oxidation of NPs. To control the size of the Bi₂Te₃ NPs and prevent surface oxidation, we employed TOP and OA.

CONCLUSIONS

Several approaches have been used to characterize Bi₂Te₃ nanorods synthesized via thermal decomposition, and their thermoelectric properties have been examined. The conversion of single-phase Bi₂Te₃ into BiTe–Bi₂Te₃ nanocomposites with increasing TOP concentration was verified by Rietveld refinement. The stoichiometric production of Bi₂Te₃ was revealed by Raman spectroscopy, which also supports the regular decrease in the crystallite size observed in the XRD. For the first time, Bi₂Te₃ nanorods' inversion symmetry is broken by ligands. FTIR was used to investigate whether ligands were present on the surface of the as-synthesized NPs. The development of particle size with TOP concentration was examined using XRD, TEM, FESEM, and DLS. The production of ligand-capped Bi₂Te₃ with varying thicknesses was compatible with zeta potential measurements. Together with electrical resistivity and Hall measurements, thermopower analysis verified that these nanocomposites are n-type semiconductors. Finally, the 40 nm crystallite size Bi₂Te₃–BiTe nanocomposite exhibited the highest power factor. The general conclusions of this study are briefly presented in the following chapter.

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