Correlation between microstructure and drastically reduced lattice thermal conductivity in Bi_2Te_3 /Bi nanocomposites for high thermoelectric figure of merit

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Abstract

The concept of nanocomposite/nanostructuring in thermoelectric materials has been proven to be an effective paradigm for optimizing the high thermoelectric performance primarily by reducing the thermal conductivity. In this work, we have studied the microstructure details of nanocomposites derived by incorporating a semi-metallic Bi nanoparticle phase in Bi_2Te_3 matrix and its correlation mainly with the reduction in the lattice thermal conductivity. Incorporating Bi inclusion in Bi_2Te_3 bulk thermoelectric material results in a substantial increase in the power factor and simultaneous reduction in the thermal conductivity. The main focus of this work is the correlation of the microstructure of the composite with the reduction in thermal conductivity. Thermal conductivity of the matrix and nanocomposites was derived from the thermal diffusivity measurements performed from room temperature to 150 °C. Interestingly, significant reduction in total thermal conductivity of the nanocomposite was achieved as compared to that of the matrix. A detailed analysis of high-resolution transmission electron microscope images reveals that this reduction in the thermal conductivity can be ascribed to the enhanced phonon scattering by distinct microstructure features such as interfaces, grain boundaries, edge dislocations with dipoles, and strain field domains.

Keywords: Thermoelectric; Solvothermal Reaction and Hot Pressing; Microstructure Characterization; Thermal Conductivity

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1. INTRODUCTION

Bi_2Te_3 and its derivative alloys are an important class of thermoelectric materials for refrigeration and power generation in the temperature range 200-400K [1, 2], having the highest figure of merit (ZT) ~ 1 . The thermoelectric figure of merit (ZT) defined as $ZT = S^2\sigma / (K_e + K_L)$, although has a complex interdependence between Seebeck coefficient (S), electrical conductivity (σ), electronic thermal conductivity (K_e) but lattice thermal conductivity (K_L) being an independent parameter can be tuned independently. Technological efforts in developing efficient modules for device fabrication are still restricted by insignificantly smaller ZT at room temperature that dictates thermoelectric efficiency besides parasitic losses and other device related issues. Bi_2Te_3 based thermoelectric modules offers a promising route to improve the efficiency of such devices at room temperature for its large scale application.

Several current strategies such as doping [3-6], solid solution alloying [7-11], several ideally engineered materials [12-14] and nanostructuring/nanocomposites [15-20] have been proposed and demonstrated to improve the ZT via circumventing the interdependencies of these three competing parameters by simultaneous optimization of the power factor and reduction in the thermal conductivity. Among all these strategies, nanocomposite approach has made a marked recognition in achieving high ZT of thermoelectric materials. This approach suggests that the ZT enhancement can be realized due to nanoscale size of inclusions incorporated into bulk thermoelectric matrix enhancing the density of grain boundaries and numerous interfaces which provides easy path for electrons to transport and effectively scattering of phonons at interfaces. The high concentration of grain boundaries and interfaces is expected to lower the lattice thermal conductivity of the materials. The nanocomposite materials introduce numerous interfaces in

which phonons over a large mean free path range can be scattered more effectively and preferentially than electrons, thereby reducing the lattice thermal conductivity effectively while preserving carrier mobility and electronic conduction.

In fact, theoretical calculations and experimental investigations [21-33] have also shown that in low dimensional structures the electronic transport properties can be significantly improved due to modified density of states. Moreover, incorporation of nanoscale particle in the matrix, introduces many internal interfaces which scatter phonon more effectively than electrons to reduce the thermal conductivity. Based on these facts, the enhancement in thermoelectric figure of merit could be achieved in thin film multilayers [29] and in bulk $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ nanocomposites having a laminated nanostructure [32] where a maxima in figure of merit, $ZT=1.47$ could be achieved at $\sim 450\text{K}$. Venkatasubramanian et al. [1] and Heremans et al. [29], have been able to show significant reduction in cross-plane and in-plane lattice thermal conductivity in $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ and $\text{PbTe}/\text{PbSeTe}$ superlattice structures, respectively. Phonon confinement in superlattices and nanowires can alter the phonon dispersion relation and reduces the specific heat and phonon group velocity, and thereby reduces the lattice thermal conductivity.

It is worth mentioning here that the creation of random interfaces on a nanometer scale by nanostructuring, increases phonon scattering at grain boundaries and interfaces, and thereby reduces the phonon mean free path for effective reduction in lattice thermal conductivity. These nanoinclusions embedded into thermoelectric matrix, grain size reduction, and creation of grain boundary interfaces due to nanostructuring can also lead to significant micro structural modifications of the bulk matrix for reduction in lattice thermal conductivity. Such reduction in the lattice thermal conductivity enhances the thermoelectric figure of merit which has been

reported by Poudel et al.[23] and Ma et al. [27]. Significant enhancement in ZT is also reported in LAST [25] system, due to the embedded quantum nanodots into the matrix structures, which modifies the micro structural features at nanoscale for effective phonon scattering and hence reduces the lattice thermal conductivity. These nanostructures were fabricated by encapsulating the nanodots into matrix by melt quenching method. Similar approach was also adopted in other systems like NaPbmSbTe_{2+m} and $\text{Pb}_{9.6}\text{Sb}_{0.2}\text{Te}_{10-x}\text{Se}_x$ [33, 34]. Incorporation of nanopowders (insulators, metals, semiconductors) or presence of nanosized cavities, into bulk thermoelectric materials has also been reported in several investigations[35-37, 39-40] in which effective phonon scattering has been taken place to reduce the lattice thermal conductivity.

Improved materials for thermoelectric applications require that the lattice thermal conductivity be reduced while retaining favorable electronic properties. The present study aims to further improve the understanding of the correlation between microstructure and lattice thermal conductivity in nanocomposites. The electronic properties of Bi_2Te_3 / Bi nanocomposites have been reported earlier in detail by our group [41]. However, in this work, we have investigated microstructural modifications of Bi_2Te_3 nanocomposites with Bi nanoinclusions on the reduction in the lattice thermal conductivity. Here, Bi has been synthesized by low temperature solvothermal route while Bi_2Te_3 has been synthesized by planetary ball milling. Finally the chemically-synthesized Bi nanoparticles were mixed in Bi_2Te_3 matrix and subsequently densified at 200 °C and 100 MPa employing conventional hot pressing technique. The melting point of the matrix ensures retention of nanostructures, grain boundary interfaces and nanograins for significant phonon scattering, compared to micron sized grains if hot pressed at high temperatures. Since transmission electron microscopy provides an appropriate means to characterize microstructural details on the nanometer scale, we report the distinct microstructure

features present in these nanocomposites (with Bi nanoinclusions), which have helped in significantly reducing the lattice thermal conductivity. Aim of this article is to correlate the compositional inhomogeneties and microstructural features in these nanocomposites with the reduction in lattice thermal conductivity. The detailed synthesis procedure of the nanocomposites and the thermoelectric transport properties was reported in [42].

2. EXPERIMENTAL

Bi nanoparticles used as nanoinclusions in this study were synthesized by a low temperature solvothermal method. BiCl_3 was used as precursor and citric acid as a surface modifier, and these constituents were weighed in 1:5 molar ratios and dissolved in 40 mL of DMF used as reducing agent. The solvent was further transferred into a Teflon lined autoclave and heated at 160°C for 6 hrs. Bi_2Te_3 composition was synthesized by planetary ball milling using Bi and Te elemental shots in 2:3 ratio. The Bi and Te shots of 5N purity (ESPI metals) were weighed in an Ar filled glove box, sealed in a stainless steel vial and subjected to ball milling for 25 hrs. The Bi and Bi_2Te_3 nanoparticles crystallized in rhombohedral symmetry (R-3m) and the phase purity was matched with the JCPDS data set of (015-0863) and (005-0519) respectively. The Bi_2Te_3 matrix phase and Bi (3% and 5%) nanoparticles incorporated Bi_2Te_3 nanocomposites, were uniaxially hot pressed at 200°C and 100 MPa. The pellets could be densified upto ~95% theoretical density. Thermal diffusivity of these samples were measured using the laser flash apparatus (Netzsch LFA-457) from RT to 150°C and the total thermal conductivity was calculated from the formula $K=D.C_p.\rho$ (where D is thermal diffusivity, C_p is specific heat and ρ is the geometrical density of the pellet). The electronic component of thermal conductivity was further calculated from the relation $K_e=L\sigma T$ (Lorentz number was taken as $L= 2.45\times 10^{-8} \text{ W}\Omega\text{K}^{-2}$). The

error in thermal conductivity measurement on Netzsch LFA-457 is within $\pm 3\%$. Room temperature Hall Effect and electrical conductivity measurements were carried out using a five-point probe method on bar-shaped samples. The sample was placed between the poles of a laboratory electromagnet which applied magnetic fields of ± 0.5 T. Longitudinal and transverse voltages were measured using an A.C. resistance bridge operating at a frequency of 13 Hz. The electrical conductivity was derived from the longitudinal potential difference and the Hall coefficient, R_H was derived from the transverse potential difference, $R_H = \frac{tV_y}{B_z I_x}$ where t is the sample width, V_y is the measured transverse voltage, B_z is the external magnetic field and I_x is the applied current. The carrier concentration is found from $n = \frac{1}{e R_H}$ where e is the fundamental electronic charge, so that the sign of the Hall coefficient gives the sign of the charge carriers. Finally, the Hall mobility μ_H was calculated by a relation $\mu_H = \sigma / n e$ where σ is the electrical conductivity. The microstructures were investigated using scanning electron microscope (JEOL-JSM) operated at 20 KV, and also by transmission electron microscope (JEOL-2010) operated at 200 KV. Elemental analysis using EDAX technique was carried out on both scanning electron and transmission electron microscope. For characterization by scanning electron microscope (SEM), the hot pressed bulk specimens were mechanically polished to a mirror finish and were chemically etched using 1:1 HNO_3 and H_2O solution. TEM specimen were prepared from the bulk by dicing 3 mm discs with an ultrasonic disc cutter (model 170, Fischione), mechanical polishing using dimple grinder with a load of 13 gm (Gatan 1656), and Ar^+ ion-milling (FISCHIONE 1010). The ion milling was done in a cold stage maintaining the temperature of -110°C in two steps. The sample was milled for two hours at 3.5 kV and 5 mA at milling angle of

10^0 to perforation followed by milling for 30 minutes at 1kV and 5mA at an angle of 8^0 . For the characterization of Bi_2Te_3 and Bi nanoparticles by TEM, suspensions of the powders in alcohol were dropped onto a holey carbon grid.

3. RESULTS AND DISCUSSION

3.1. Electron microscopy studies on the matrix Bi_2Te_3 and Bi/ Bi_2Te_3 nanocomposite.

The Bi nanoparticles synthesized by solvothermal method have a wide particle size distribution with particles ranging in size from 10-200 nm, but majority of particles in size ranging from 20-80 nm. The representative TEM image of Bi nanoparticles is shown in Figure 1(a) and the particle size distribution histogram (generated from the statistical size distribution analysis on TEM images from different areas of one sample) is shown as an inset in Figure 1(a). The Bi nanoparticles crystallize in rhombohedral (space group $R\bar{3}m$, 166) symmetry, with lattice parameters $a=4.546 \text{ \AA}$; $c=11.860 \text{ \AA}$, and the particles adopt a spherical shape. Some particles are faceted, as illustrated in Fig. 1(b) and a particle is shown in $\langle 110 \rangle$ orientation, exhibiting (001) and (101) surface planes. The corresponding (003) and (101) lattice planes are clearly resolved, illustrating the excellent crystallinity of the bismuth nano-particles. The excellent crystallinity of Bi nanoparticles can also be seen in Figures 1(c) and 1(d). In Figure 2(a), the scanning electron micrographs of the consolidated matrix (Bi_2Te_3) phase is shown and it is compared with the SEM image of the 5 % Bi incorporated Bi_2Te_3 nanocomposite, shown in Figure 2(b). In the matrix phase shown in Figure 2(a), more elongated and irregular shaped grains with bi-modal size distribution were observed. The EDAX obtained from the SEM on ball milled Bi_2Te_3 shown in Figure 2(c), clearly indicates the presence of Bi and Te. The quantification obtained from SEM-EDAX spectrum shown in the inset of Fig 2(c) revealed the composition to be very close to the

nominal composition. Figure 2(b) displays the SEM image corresponding to the sample of 5 % Bi incorporated Bi_2Te_3 composite. Interestingly, large matrix grains of the composite material at high magnification shown in the inset of Figure 2(b) presents dispersion of small white contrast particles marked by arrow in the grain matrix. The EDAX analysis shown in fig 2(d) obtained from the white contrast particle clearly confirms the presence of Bi nanoparticles indicating the Bi distribution in Bi_2Te_3 matrix. The density of the matrix and nanocomposites used in this work are about 95% as compared to the respective theoretical densities of these samples, but some amount of porosity could be observed from in the matrix phase compared to nanocomposite. The geometrical density of the matrix and nanocomposites is given in table 1.

In order to understand the internal structure of matrix and nanocomposite materials, the transmission electron microscopy has been performed. Figure 3(a) displays bright field electron micrograph of the as synthesized powder of Bi_2Te_3 sample. The size of synthesized powder particles of Bi_2Te_3 was observed to be ranging from 10 nm to 40 nm, envisaged from fig 3(a). Figure 3(b) presents the TEM image obtained from the hot pressed densified sample of Bi_2Te_3 . A clear grain growth was observed during hot pressing and it ranges from 64 nm to 0.4 μm (figure 3(b)). As seen in Figure 3(b) the grain growth results in a densified structure and fine grain boundary interfaces, which is essential for phonon scattering. Bi_2Te_3 has a rhombohedral structure with lattice parameters $a = 4.43 \text{ \AA}$ and $c = 29.91 \text{ \AA}$, and Figure 3(c) shows the selected area diffraction (SAED) pattern indexed in the rhombohedral unit cell seen along the $[1 -1 0 -1]$ zone axis orientation. Bi_2Te_3 is also a layered structure and Figure 3(d) shows the layering and resolved lattice planes along the c-axis, viewed on one of the grains in Figure 3(b). The corresponding SAED seen in the inset of Figure 3(d) confirms the stacking of lattice planes along c-axis. The antisite defect structure in Bi_2Te_3 is also well known and as a result of ball milling technique,

compositional variation and inhomogenities could be observed in the matrix Bi_2Te_3 (free of inclusions). In Figure 4(a), a Te rich particle is observed at the intersection between the three grains. The region highlighted by a rectangle is a Te rich region together with insignificant amount of Bi and EDAX confirms 98.76 at% Te, and extra half planes extend from the Te rich side towards the interface with the matrix phase indicating that the precipitate is semi-coherently embedded ($r_0 < \text{Te} < r_0 \text{ Bi}$), see arrows in Fig.4 (b). The compositional fluctuations creating atomic scale defects such as Te rich helps in scattering of short wavelength phonons and thereby resulting in reducing the thermal conductivity. An enlarged view of a grain which is shown in Figure 4(c) indicates highly strained lattices generating misfit type of dislocations (enlarged view inset fig 4c) along (0 1 5) direction as marked by closed loop. The Fast Fourier transform (FFT) (inset Fig 4c) obtained from the region marked by loop also confirms the dislocation plane to be in the direction of (0 1 5) plane. In Bi_2Te_3 system, the point defects due to the intrinsic antisite defect structure, line dislocations like edge dislocation and stacking fault are inherently present and a low temperature hot pressing (200°C) is not sufficient to anneal all the defects.

With 5% (volume fraction) Bi nanoparticle incorporation, we observe an uneven distribution of Bi nanoparticles throughout the grain matrix, and no preference along the grain boundaries could be detected. We find regions with fine dispersion of Bi nanoparticles and regions devoid of these inclusions, as shown in Figure 5(a) and a magnified image of the region with Bi nanoparticles is seen in the inset. The presence of the Bi nanoinclusions (marked as A) located on the grain matrix (marked as B) is seen in Figure 5(b) which is confirmed by EDAX-TEM analysis. Fig 5(c) presents the EDAX spectra corresponding to region A and B confirming the region A containing only Bi peaks while the spectrum from region B contains the elemental peaks of both Bi and Te. The quantification of EDAX spectrum from regions A and region B (which is not shown here)

confirms the composition of Bi and Bi_2Te_3 stoichiometries respectively. The region A and region B were examined by EDAX-TEM analysis and are confirmed to be Bi nanoparticles from EDAX spectra and the region B which is the matrix phase consisting of both Bi and Te as evident by Fig 5(c). In order to confirm the inclusion A to be Bi particle, the FFT was performed and was found to be well indexed with Bi; rhombohedral structure with lattice parameters; $a = 4.53 \text{ \AA}$ and $c = 11.84 \text{ \AA}$ along the zone axis of $[1 \ -1 \ 0 \ 0]$ presented in Fig 5(d). The inverse FFT (Fig 5e-f) has also been performed corresponding to g_{11-20} and g_{000-6} showing excellent crystallinity along $(1 \ 1 \ -2 \ 0)$ and $(0 \ 0 \ 0 \ -6)$ planes of Bi respectively. Thus, evidently, the Bi nanoinclusions were found to be resided within the grain matrix of Bi_2Te_3 . The nanoinclusions of Bi provide additional scattering centers for the phonons to scatter other than grain boundaries which will be discussed in the forthcoming part of the manuscript.

Apart from the nanoprecipitates and defects, strain field domains could be seen in some regions of the specimen. An antiphase boundary between two domains and a (π) phase shift between these domains causes strain fields, which can be imaged by HRTEM and is commonly observed in ferroelectrics [43]. Evidence of strain field domains in n and p type Bi_2Te_3 has been reported by D. Maier [44]. We have also been able to observe these strain field domains in the 5% Bi incorporated Bi_2Te_3 nanocomposites also, as shown in Figure 6(a). Only under some diffraction conditions $g = (-1, 0, 5)$ with zone axis close to the $[010]$ pole, these features could be observed as shown in Figure 6(a), and these strain field domains are visible as black and white stripes, with periodicity of 3 nm. The cause for the strain fields was further imaged by HRTEM in $[010]$ zone axis shown in Figure 6(b) and the FFT is shown in the inset (Figure. 6 (b)). An inverse Fourier transform by digital Micrograph software, further generated the lattice fringe image with $(-1, 0, 5)$ spot, as shown in Figure 6(c). The lattice fringe image shows the edge dislocations originated

from the relaxation of the strain field. It is proposed by D. Maier [44] that such a strain field domain in thermoelectric materials can cause some changes in band structure and create shallow potential superlattice similar to the superlattice structure in $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ [1], for scattering of acoustic phonons which are the major carriers of heat in a material.

3.2. Thermal conductivity in Bi_2Te_3 and Bi/ Bi_2Te_3 nanocomposite

The total thermal conductivity (κ) is the product of thermal diffusivity, specific heat (shown in supplementary fig S2 & S3) and density (table 1). The lattice thermal conductivity (κ_l) was estimated by subtracting the electronic contribution (κ_e) from the total thermal conductivity (κ). The electronic contribution to the thermal conductivity (κ_e) can be estimated using the Wiedemann-Franz law (i.e. $\kappa_e = L \sigma T$, where L is Lorenz number, σ , the electrical conductivity and T , the temperature in K). Here, we use the temperature dependent Lorenz number [45] and the bipolar contribution was taken into account by assuming $\kappa_{\text{lattice}} \sim T^{-1}$ [46]. Figure 7(a-b) present the total thermal conductivity coupled with lattice thermal conductivity and the electronic thermal conductivity respectively. It can be seen in Figure 7(a) that with the addition of Bi nanoparticle the total thermal conductivity decreases and for a 5% Bi incorporated nanocomposite the thermal conductivity is the least. The lattice thermal conductivity shown in the same graph shows a reduction with the Bi nanoparticle incorporation. The decrease in lattice thermal conductivity overrides the increase in electronic thermal conductivity. Interestingly, the thermal conductivities of the present composites at room temperature were observed to be much smaller than that of state-of-the-art Bi_2Te_3 based materials [27, 33], as evidenced in Figure 7(c). Further, in order to check the thermal stability of nanocomposites, the retraceability of thermal conductivity was verified during heating and cooling experiments which is shown in the supplementary information

S1. From figure S1, the variation in thermal conductivity values during heating and cooling can be noted to have minimal changes suggesting the nanocomposites to be thermally stable.

The increase in electronic thermal conductivity shown in Figure 7(b) is due to an increase in carrier concentration with Bi nanoinclusions which is evidenced by Hall data shown in table 1. From Hall measurements we deduced that the carrier concentration increases from $1.7 \times 10^{19}/\text{cm}^3$ to $3.1 \times 10^{19}/\text{cm}^3$ for Bi_2Te_3 (without nanoinclusions) and 5% Bi incorporated Bi_2Te_3 nanocomposite, respectively [40]. The carrier mobility in the 5% Bi nanocomposite remained very similar to matrix phase resulting in a significant increase in the electrical conductivity and hence the electronic component of the thermal conductivity. However, the mobility for the 3% Bi nanocomposite was reduced by 26% resulting in an electrical conductivity (and electronic thermal conductivity) only slightly larger than the Bi_2Te_3 without nanoinclusions near room temperature. We understand that the reduction in lattice thermal conductivity of the present composite is due to combined effect of primarily varying particle sizes and grain boundaries relating to models described by Goldsmid [47] and Toberer et al. [48], and several microstructural phenomena such as strain field domain, edge dislocations and multiple grain boundaries. As discussed by Maier et al., the major carriers of heat i.e. acoustic phonons are scattered at these domains and consequently the lattice thermal conductivity is lowered as shown in Fig 7(a). Thus present nanocomposites fabricated by Bi incorporation in Bi_2Te_3 leads to significant reduction in thermal conductivity due to phonon scattering not only at grain boundaries and interfaces but several microstructure disorder such as dislocations strain field and defects for effective phonon scattering covering short to high wavelength phonon.

4. CONCLUSIONS

In summary, we have carried out a detailed microstructure investigation of Bi_2Te_3 matrix phase and a 5% (volume fraction) Bi incorporated Bi_2Te_3 nanocomposite. The Bi nanoinclusions are seen to be embedded inside the grain matrix and these nanoparticles and nanoprecipitates create additional phonon scattering centers for significant reduction in lattice thermal conductivity. The presence of line imperfections (like edge dislocations and stacking faults), strain field domains present in the nanocomposites also interact with optical/acoustic phonons for reduction in lattice thermal conductivity. The wide particle size distributions of the Bi nanoinclusions in the composites help in a wide range of phonon wavelengths scattering. While nanograins of Bi_2Te_3 matrix phase provide many internal interfaces for scattering of short wavelength phonons. Hence we conclude that a combined effect of nanoparticles as a secondary phase and presence of nanograins helped in reduction in lattice thermal conductivity inspite of an increase in electronic thermal conductivity, for an overall reduction in total thermal conductivity with Bi nanoinclusions.

5. ACKNOWLEDGEMENTS

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Figure 1: (a) Bright field TEM image of Bi nanoparticles synthesized by solvothermal method and (b-d) HRTEM images of Bi nanoparticles showing excellent crystallinity.

Figure 2: (a) SEM image of hot pressed sample of Bi_2Te_3 matrix phase; inset is EDAX-SEM spectrum from matrix phase (b) SEM image obtained from 5 vol% Bi/ Bi_2Te_3 composite (c) EDAX-SEM spectrum from matrix phase (d) EDAX-SEM spectrum from Bi particle dispersed in matrix.

Figure 3: (a-b) Bright field TEM images taken from starting powder sample of Bi_2Te_3 matrix and hot pressed sample respectively ; (c) SAED pattern correspond to Bi_2Te_3 grain matrix (d) A perfect layering of Bi_2Te_3 and SAED pattern (inset: Fig 3d) corresponding to layered structure showing stacking of lattice planes along the c axis.

Figure 4. (a-c) Bright field TEM images obtained from Bi_2Te_3 matrix showing a chemical inhomogenities.

Figure 5: (a) Bright field TEM images taken from $\text{Bi}_2\text{Te}_3/\text{Bi}$ composite showing dispersion of Bi nanoparticles in Bi_2Te_3 matrix (b) enlarged region of a matrix grain B is shown together with an inclusion of Bi (marked 'A') (c) EDAX, TEM spectrum from region A and region B (fig. 5(b) showing inclusion of Bi phase and Bi_2Te_3 matrix phase respectively (d) The fast Fourier transform (FFT) obtained from region A was indexed with rhombohedral structure of Bi along the zone axis of $[1\ -1\ 0\ 0]$. (e-f) The inverse FFT corresponding to $g_{1\ 1\ -2\ 0}$ and $g_{0\ 0\ 0\ -6}$ showing excellent crystallinity along $(1\ 1\ -2\ 0)$ and $(0\ 0\ 0\ -6)$ planes of Bi respectively.

Figure 6: (a) Low magnification bright field TEM image of the strain field domain structure under the diffraction condition $g = (-1, 0, 5)$ with zone axis close to the $[0\ 1\ 0]$ pole (b) HRTEM image in the $[0\ 1\ 0]$ pole (c) Inverse Fourier- transformation of $(-1\ 0\ 5)$ spot. Edge dislocations, which are part of domains, are indicated by arrows. These dislocations are mostly dipoles that are about 1.5 nm

Figure 7: (a) Total and lattice thermal conductivity in Bi_2Te_3 and Bi (3% and 5%) incorporated Bi_2Te_3 nanocomposites. Open legends correspond to total thermal conductivity and closed legends correspond to lattice thermal conductivity. NC refers to nanocomposite with Bi nanoinclusions. (b): Electronic thermal conductivity in Bi_2Te_3 and Bi (3% and 5%) incorporated Bi_2Te_3 . (c) Total thermal conductivity compared to literature data for p-type materials. Poudel (2008) [33], Ma-I (2008)[27] nanostructured $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$ made from a commercial ingots, Ma-E (2008)[27] nanostructured $\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$ made from elemental constituents. The minimum thermal conductivity for the n-type materials from this study is similar to the minimum thermal conductivity of the p-type materials, but shifted to lower temperature.

Table1. Various room temperature physical parameters for Bi₂Te₃ and Bi/Bi₂Te₃ nanocomposites

Sample Name	Hall Coefficient	Resistivity	Carrier Concentration	Carrier Mobility	Seebeck Coefficient	Density
	(cm^3 / C)	($\Omega .cm$)	($\times 10^{19} cm^{-3}$)	($cm^2 / V^I s^{-I}$)	($\mu V / K$)	(g/cm^3)
Bi ₂ Te ₃	-3.78×10^{-1}	5.20×10^{-3}	1.652	72.607	178	7.060
Bi/Bi ₂ Te ₃ (3% Bi NC)	-2.92×10^{-1}	4.35×10^{-3}	2.653	54.044	167	7.726
Bi/Bi ₂ Te ₃ (5% Bi NC)	-2.03×10^{-1}	2.76×10^{-3}	3.08	73.297	171	7.624

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

FIGURE 7