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Supplementary Information

Enhanced Thermoelectric Performance of Bi-Sb-Te/Sb_2O_3 Nanocomposites by Energy Filtering Effect

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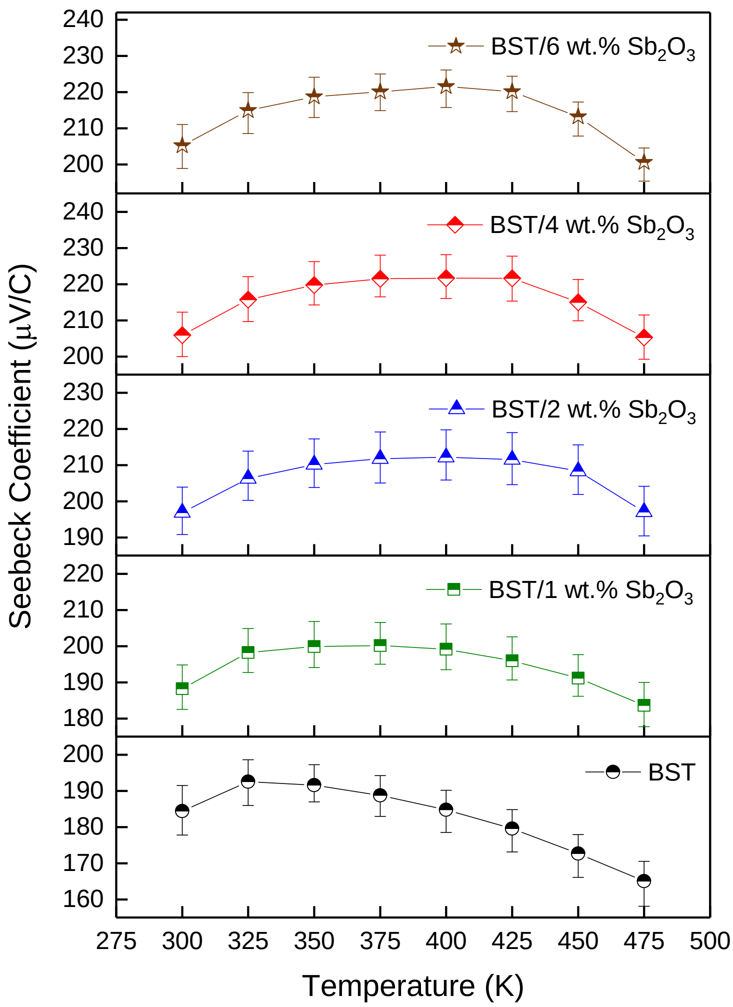

Figure S1. Seebeck coefficient variation with temperature.

Figure S1 shows the Seebeck coefficient (*S*) variation of p-type BST and its composites with Sb_2O_3 nanoparticles measured between 300 K and 475 K. The symbols in each case represent the sample with intermediate *S* values, and the error bars represent the samples with minimum and maximum S values.

It is known that by using Boltzmann transport theory and the single parabolic band (SPB) model approximation, the Seebeck coefficient and charge carrier concentrating can be expressed as:

$$S(\eta) = \frac{k_B}{q}\left[\frac{(r+5/2)F_{(r+3/2)}(\eta)}{(r+3/2)F_{(r+1/2)}(\eta)} - \eta\right] \tag{1}$$

$$p_H = 4\pi\left(\frac{2m^* k_B T}{h^2}\right)^{3/2} F_{(1/2)}(\eta) \tag{2}$$

$$F_i(\eta) = \int_0^\infty \frac{x^i dx}{1+\exp(x-\eta)} \tag{3}$$

where η is the reduced Fermi level, k_B is the Boltzmann constant, q is the elementary charge, r is the scattering parameter, R_H is the Hall coefficient, m^* is the density of state effective mass, T is the absolute temperature, and ħ is the reduced Planck constant. When charge carriers are scattered by acoustic phonons, we can assume r = – ½ in Equation (1).

By considering the pure BST sample at room temperature as the reference sample, a density of state effective mass of $m^* = 1.25m_0$ is obtained from Equations (1-3), in which m_0 is the mass of an electron. To evaluate if the improvement of Seebeck coefficient in nanocomposite samples can be related to "energy filtering effect" or not, the obtained m* in pure BST will be considered as constant for all other samples. Then by substituting the carrier concentration (P_H) values in Equation (2) and considering r = – ½ at room temperature $F_{(1/2)}(\eta)$ is calculated for those samples. Then using Equation (3), η is calculated, and finally using Equation (1), the Seebeck coefficient is calculated, as shown in Table 1.

Table 1. A comparison between the Seebeck coefficient of BST/Sb_2O_3 samples and the calculated values, supposing there was no energy filtering effect.

Sample	Measured carrier concentration (1/m^3)	Measured Seebeck Coefficient (μV/K)	Calculated Seebeck Coefficient (μV/K)
Pure BST	3.50647 (10^{25})	184.4	184.4
BST/1 wt.% Sb_2O_3	3.01522 (10^{25})	188.2	195.9
BST/2 wt.% Sb_2O_3	2.38226 (10^{25})	196.9	214.2
BST/4 wt.% Sb_2O_3	2.20548 (10^{25})	205.9	220.2
BST/6 wt.% Sb_2O_3	2.467 (10^{25})	205.2	211.4

It is noticed that the calculated Seebeck coefficients have different values from the measured Seebeck coefficients in BST/Sb_2O_3 nanocomposite samples. Therefore, we can conclude that the increase of the Seebeck coefficient by adding Sb_2O_3 nanoparticles cannot only be attributed to the change in carrier concentration of the samples. Thus, it is reasonable to assume the influence of energy filtering on the Seebeck coefficient of the composites.

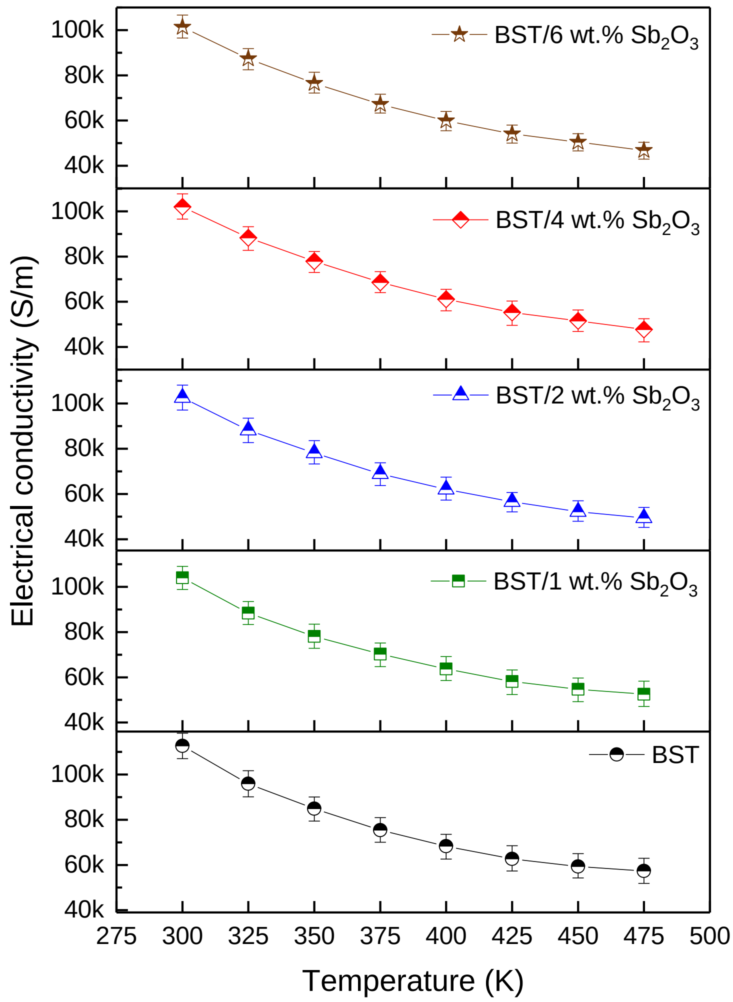

Figure S2. Electrical conductivity variation with temperature.

Figure S2 shows the electrical conductivity (σ) variation of p-type BST and its composites with Sb_2O_3 nanoparticles measured between 300 K and 475 K.

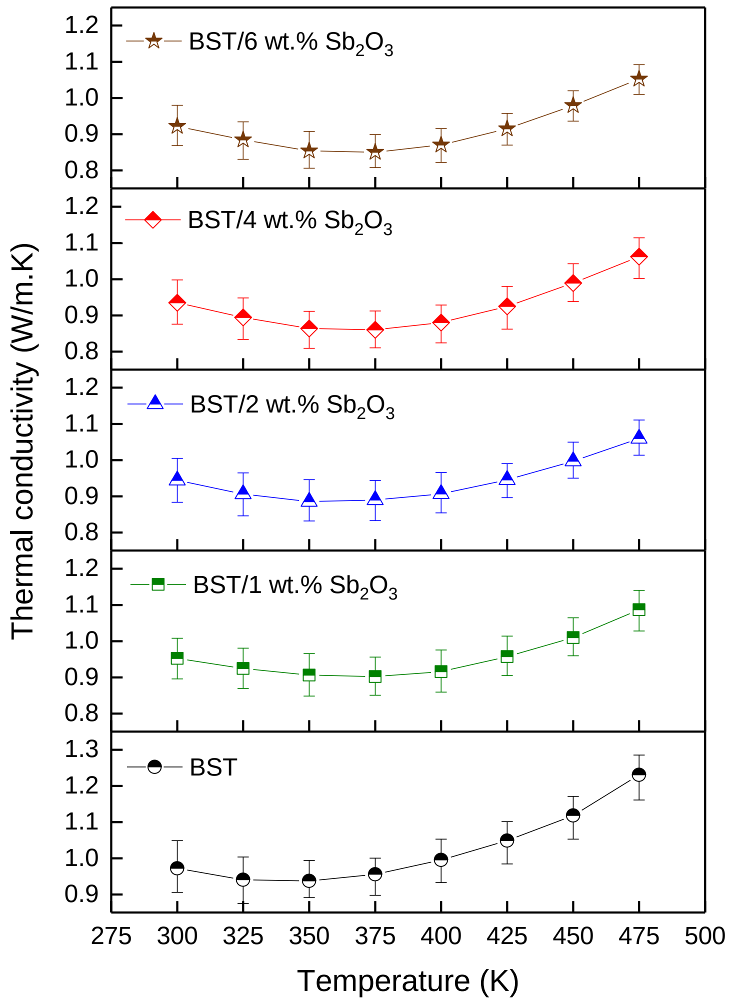

Figure S3. Thermal conductivity variation with temperature.

Figure S3 shows the thermal conductivity (K_{tot}) variation of p-type BST and its composites with Sb_2O_3 nanoparticles measured between 300 K and 475 K.