Electronic Supplementary Information (ESI)

Enhancing thermoelectric performance of N-type Bi$_{2}$Te$_{2.7}$Se$_{0.3}$ through incorporation of Ag$_{9}$AlSe$_{6}$ inclusions

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1. The measured densities for all the bulk samples

Table S1 The density\( (d) \) and the relative density\( (d_r) \) of BTS-xvol%Ag\(_9\)AlSe\(_6\) \((x=0, 0.15, 0.25, 0.35, 0.50\) and 0.70). 

<table>
<thead>
<tr>
<th>Bi(<em>2)Te(</em>{2.7})Se(_{0.3}) -xvol. % Ag(_9)AlSe(_6)</th>
<th>(d) (g cm(^{-3}))</th>
<th>(d_r) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x=0)</td>
<td>7.82</td>
<td>98.9</td>
</tr>
<tr>
<td>(x=0.15)</td>
<td>7.78</td>
<td>98.4</td>
</tr>
<tr>
<td>(x=0.25)</td>
<td>7.83</td>
<td>99.0</td>
</tr>
<tr>
<td>(x=0.35)</td>
<td>7.76</td>
<td>98.1</td>
</tr>
<tr>
<td>(x=0.50)</td>
<td>7.79</td>
<td>98.5</td>
</tr>
<tr>
<td>(x=0.70)</td>
<td>7.69</td>
<td>97.3</td>
</tr>
</tbody>
</table>

where \(d_r\) is relative density, defined as \(d_r = d/d_o\), here \(d\) is the measured density and \(d_o\) (7.91 of g cm\(^{-3}\)) is the theoretical density of Bi\(_2\)Te\(_{2.7}\)Se\(_{0.3}\). For composite specimens Bi\(_2\)Te\(_{2.7}\)Se\(_{0.3}\) -xvol. % Ag\(_9\)AlSe\(_6\), the theoretical density is modified as: \(d_o = (1-x) d_1 + x d_2\), where \(d_1 = d_o\) for BTS matrix and \(d_2\) (7.14 g cm\(^{-3}\)) is the theoretical density of Ag\(_9\)AlSe\(_6\).
2. SEM image of the BTS

FIG.S1. SEM image of the fractured surface of the BTS.

3. SEM image of the Ag$_9$AlSe$_6$ particle

FIG.S2. SEM image of the Ag$_9$AlSe$_6$ particle.
4. SEM and EDS images of fracture surfaces of the bulk sample BTS-0.35Vol%Ag9AlSe6

![SEM and EDS images](image)

FIG. S3. SEM and EDS images of fracture surfaces of the bulk sample BTS-0.35Vol%Ag9AlSe6.

5. The dependence of absolute Seebeck coefficient $S$ on carrier concentration (Pisarenko curve)

![Pisarenko curve](image)

FIG. S4. The dependence of absolute Seebeck coefficient $S$ on carrier concentration (Pisarenko curve) at 300 K and 370K for BTS-xvol%Ag9AlSe6 ($x=0$, 0.15, 0.25,
6. The temperature dependence of thermal conductivity of electric component $\kappa_E$

FIG.S5. The temperature dependence of thermal conductivity of electric component $\kappa_E$ for BTS-$x$vol$\%$Ag$_9$AlSe$_6$ ($x$=0, 0.15, 0.25, 0.35, 0.50 and 0.70).
7. The thermal stability for BTS-0.35vol%Ag$_9$AlSe$_6$ sample

FIG.S6. The cyclic measurements for the BTS-0.35vol%Ag$_9$AlSe$_6$ sample. Temperature-dependent (a) Seebeck coefficient, (b) electrical resistivity, (c) total thermal conductivity and (d) ZT, wherein the symbol 1st Heating and Cooling, 2nd Heating and Cooling stand for the first heating and cooling, second heating and cooling measurements.

8. Calculation of Lattice Thermal Conductivity

The lattice thermal conductivity $\kappa_L$ can be calculated by using the Debye-Callaway model[1]:

$$
\kappa_L = \frac{4\pi k_B^2 T^3}{\nu h^3} \tau_D \int_0^{\theta_D} \frac{z^4 \text{exp}^\infty(z)}{[\exp(z) - 1]^2} dz
$$

(S1)

$$
\tau^{-1} = \tau_U^{-1} + \tau_N^{-1} + \tau_{PD}^{-1} + \tau_{E}^{-1} + \tau_{B}^{-1} + \tau_{NP}^{-1}
$$

(S2)

where $\tau_U$, $\tau_N$, $\tau_{PD}$, $\tau_E$, $\tau_B$ and $\tau_{NP}$ are relaxation time corresponding to the scattering from phonon-phonon U- and N-process (U+N), point defects (PD), electron-phonon (E), phase boundaries (B), and nanoparticles (NP), respectively. Here, this model is used to analyze the lattice thermal conductivity. To analyze the $\kappa_L$ the expression of the
different scattering mechanisms can be rewritten as below:

$$\tau^{-1}_U = \frac{h\gamma^2\omega^2 T - \theta_D/3T}{Mv^2\theta_D} e^{-\theta_D/3T}$$  \hspace{1cm} (S3)

$$\tau^{-1}_N = \beta \tau^{-1}_U = \frac{h\gamma^2\omega^2 T - \theta_D/3T}{Mv^2\theta_D} e^{-\theta_D/3T}$$  \hspace{1cm} (S4)

$$\tau^{-1}_{PD} = \frac{V\omega^4}{4\pi v^3\Gamma}$$  \hspace{1cm} (S5)

$$\tau^{-1}_E = \frac{E_{def} m^* \omega^2}{2\pi\hbar^3\rho v}$$  \hspace{1cm} (S6)

$$\tau^{-1}_B = v/l$$  \hspace{1cm} (S7)

$$\tau^{-1}_{NP} = v\left[(2\pi R)^2 + \left(\frac{4\pi R^2(\Delta D/D)^2(\omega R)^4}{9}\right)^{-1} N_p\right]^{-1}$$  \hspace{1cm} (S8)

$$A = \frac{V}{4\pi v^3\Gamma}$$  \hspace{1cm} (S9)

$$B = (1 + \beta) \frac{h\gamma^2}{Mv^2\theta_D}$$  \hspace{1cm} (S10)

$$C = \frac{E_{def} m^*}{2\pi\hbar^3\rho v}$$  \hspace{1cm} (S11)

Thus

$$\tau^{-1} = A\omega^4 + B\omega^2 T e^{\left(-\theta_D/3T\right)} + C\omega^2 + v/l + v\sigma N_p$$  \hspace{1cm} (S12)

To quantitatively calculate $\kappa_L$, the literature values $\theta_D=164K$ and sound velocity $v=1778m/s$ are used for BTS - xvol% Ag$_9$AlSe$_6$ ($x=0, 0.15, 0.25, 0.35, 0.50$ and $0.70$). $l$ is the average spatial distance between the Ag$_9$AlSe$_6$ nanoparticles in the BTS, $\Delta D/D = 0.022$ and the average radius of Ag$_9$AlSe$_6$ $R = 628$ nm; the pre-factors of point defect A, U- and N- process B, electron-phonon scattering C and the number density of nanoparticles $N_p$ were provided in Table S2.

Table S2 Parameters for the calculation of lattice thermal conductivity by using the Debye-Callaway model

| Sample | A($10^{-42}s^3$) | B($10^{-17}sK^{-1}$) | C($10^{-16}S$) | l(nm) | $N_p(10^{13}m^{-3})$
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<tbody>
<tr>
<td>0</td>
<td>4.6</td>
<td>3.9</td>
<td>1.8</td>
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<tr>
<td>0.15</td>
<td>4.6</td>
<td>3.9</td>
<td>1.8</td>
<td>533</td>
<td>4.54</td>
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<tr>
<td>0.25</td>
<td>4.6</td>
<td>3.9</td>
<td>1.8</td>
<td>477</td>
<td>4.81</td>
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<tr>
<td>0.35</td>
<td>4.6</td>
<td>3.9</td>
<td>1.8</td>
<td>404</td>
<td>6.34</td>
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</tr>
<tr>
<td>0.50</td>
<td>4.6</td>
<td>3.9</td>
<td>1.8</td>
<td>352</td>
<td>6.83</td>
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<tr>
<td>0.70</td>
<td>4.6</td>
<td>3.9</td>
<td>1.8</td>
<td>430</td>
<td>5.37</td>
</tr>
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</table>

Reference
