Supporting Information

Thermoelectric performance of nanostructured In/Pb codoped SnTe with band convergence and resonant level prepared via a green and facile hydrothermal method

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Lorenz number calculation in details:

In general, the total (κ) consists of the electronic thermal conductivity (κ_e) and lattice thermal conductivity (κ_L). The electronic part κ_e is directly proportional to the electrical conductivity σ through the Wiedemann-Franz relation, $\kappa_e = L\sigma T$, where L is Lorentz number and its value is calculated by SPB model.[46] The Lorenz number can be given as:

$$L = \left(\frac{k_B}{e}\right)\left(\frac{(r+7/2)F_{r+5/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)} - \left[\frac{(r+5/2)F_{r+3/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)}\right]^2\right) \quad (1)$$

For the Lorenz number calculation, we should get reduced Fermi energy η firstly; the calculation of η can be derived from the measured Seebeck coefficients by using the following relationship:

$$S = \pm\frac{k_B}{e}\left(\frac{(r+5/2)F_{r+3/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)} - \eta\right) \quad (2)$$

where $F_n(\eta)$ is the $n-$th order Fermi integral,

$$F_n(\eta) = \int_0^\infty \frac{\chi^n}{1+e^{\chi-\eta}} d\chi \quad (3)$$

where e is the electron charge, k_B is the Boltzmann constant, h is the Planck constant, r is the scattering factor. The scattering factor (r) is $-1/2$ since acoustic phonon scattering has been assumed as the main carrier scattering mechanism near room temperature (RT). Lorentz number can be obtained by combining equations (1), (2) and (3).

Table S1. Sample density of pure SnTe, $Sn_{0.99}Pb_{0.01}Te$ and $Sn_{0.99-x}Pb_{0.01}In_xTe$ measured by Archimedes method.

Composition	Density [g cm-3]
SnTe	**6.171**
$Sn_{0.99}Pb_{0.01}Te$	**6.226**
$Sn_{0.98}Pb_{0.01}In_{0.01}Te$	**6.153**
$Sn_{0.97}Pb_{0.01}In_{0.02}Te$	**6.122**
$Sn_{0.96}Pb_{0.01}In_{0.03}Te$	**6.064**

Table S2. The lattice parameters extracted from the XRD Rietveld refinement for pure SnTe, $Sn_{0.99}Pb_{0.01}Te$ and $Sn_{0.99-x}Pb_{0.01}In_xTe$.

Composition	**a = b = c (Å)**	**Volume (Å^3)**
SnTe	6.32898	253.51
$Sn_{0.99}Pb_{0.01}Te$	6.33720	254.50
$Sn_{0.98}Pb_{0.01}In_{0.01}Te$	6.32921	253.54
$Sn_{0.97}Pb_{0.01}In_{0.02}Te$	6.32728	253.31
$Sn_{0.96}Pb_{0.01}In_{0.03}Te$	6.32686	253.26

Figure S1. (a, b) elemental mapping of polished surface of pure SnTe sample.

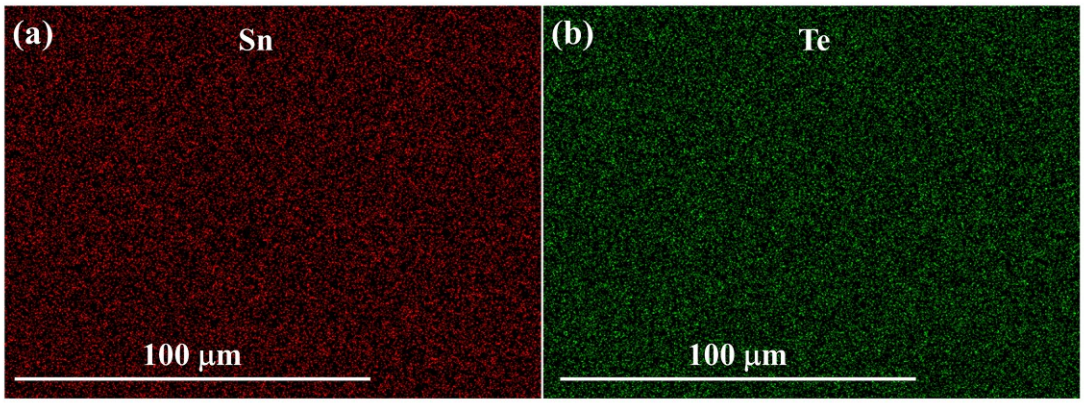

Figure S2. (a~c) elemental mapping of polished surface of $Sn_{0.99}Pb_{0.01}Te$ sample.

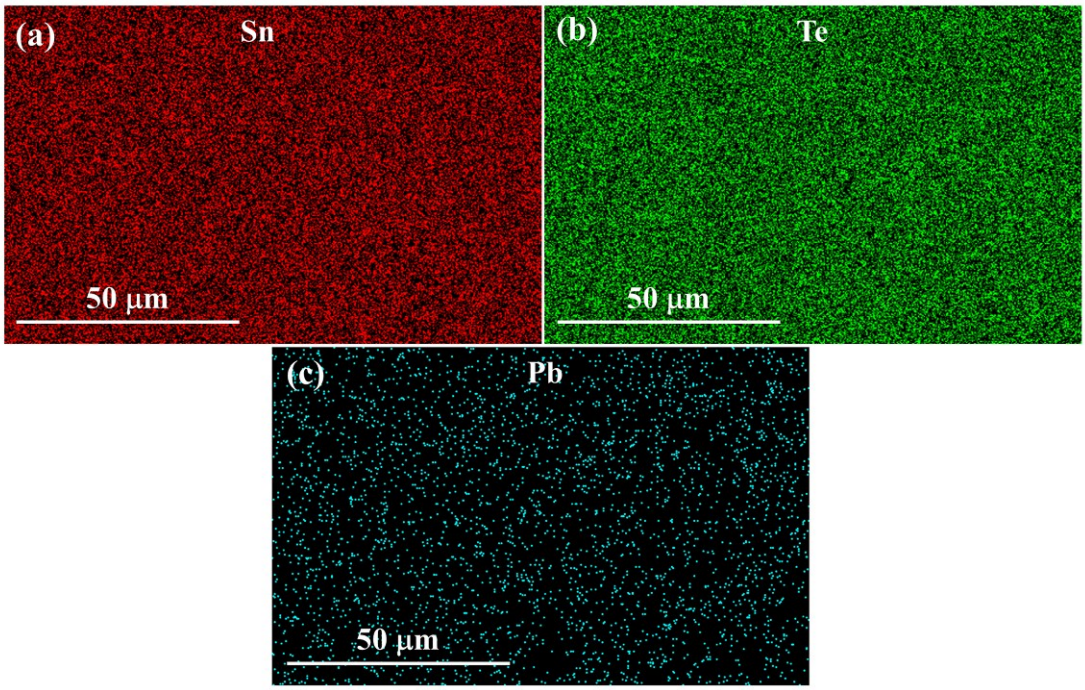

Figure S3. (a~d) elemental mapping of polished surface of $Sn_{0.96}Pb_{0.01}In_{0.03}Te$ sample.

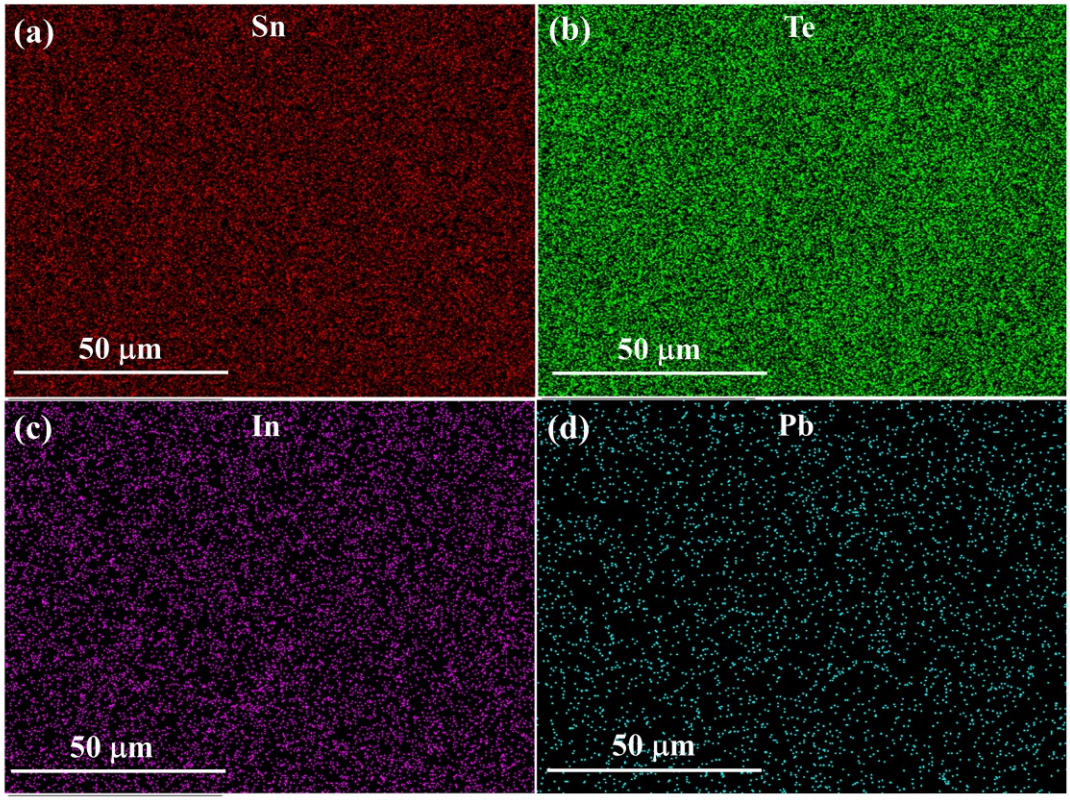

Figure S4. (a) SEM image of sintered $Sn_{0.96}Pb_{0.01}In_{0.03}Te$ sample. (b-e) Elemental mapping of $Sn_{0.96}Pb_{0.01}In_{0.03}Te$ sample marked by a red rectangle in (a).

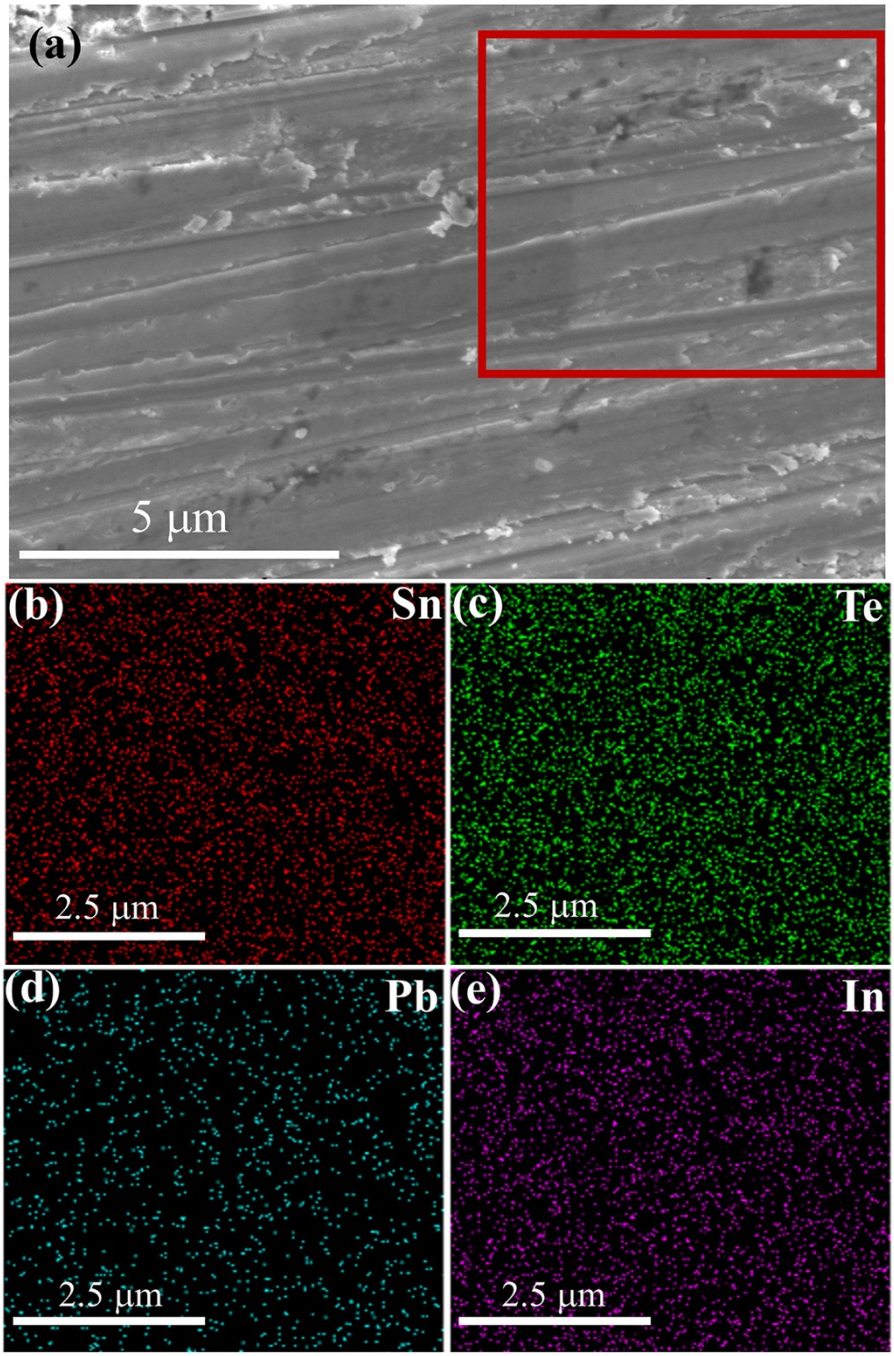

Figure S5. Temperature dependence of Lorenz number for bulk polycrystalline pure SnTe and $Sn_{0.99-x}Pb_{0.01}In_xTe$ samples.