Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Suppression of bipolar excitation and enhanced thermoelectric performance in n-type Bi_2Te_3 with argyrodite Ag_8SnSe_6 inclusion

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The analysis of preferred orientation

The degree of the grain orientation in the samples can be described by the orientation factor (F), calculated using the Lotgering method. F is defined as:

$$F = \frac{P - P_o}{1 - P_o} \qquad S1$$

$$P = \frac{I_{(00l)}}{\sum I_{(hkl)}} \qquad S2$$

$$P_o = \frac{I_{o(00l)}}{\sum I_{o(hkl)}} \qquad S3$$

where I(00l) and I_o(00l) are the intensities of XRD reflection peaks for oriented and non-oriented samples, respectively; ΣI(hkl) and ΣI_o(hkl) are the sum of the intensities of all peaks for the measured section in oriented and non-oriented samples.

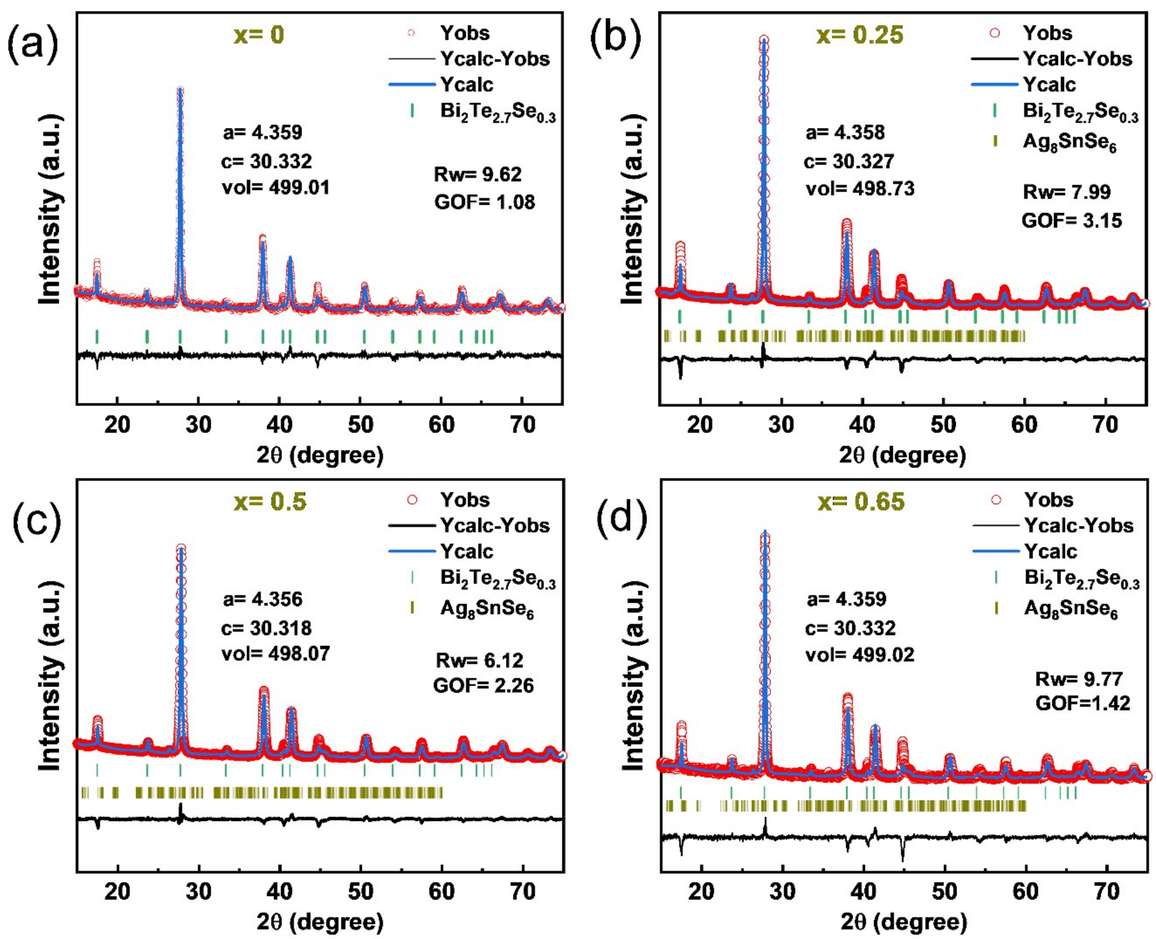

Figure. S1. Rietveld refined analysis from PXRD patterns of (a)-(d) $Bi_{1.995}Cu_{0.005}Te_{2.69}Se_{0.33}Cl_{0.03}$ + *x* wt % STSe (*x* = 0, 0.25,0.5, and 0.65).

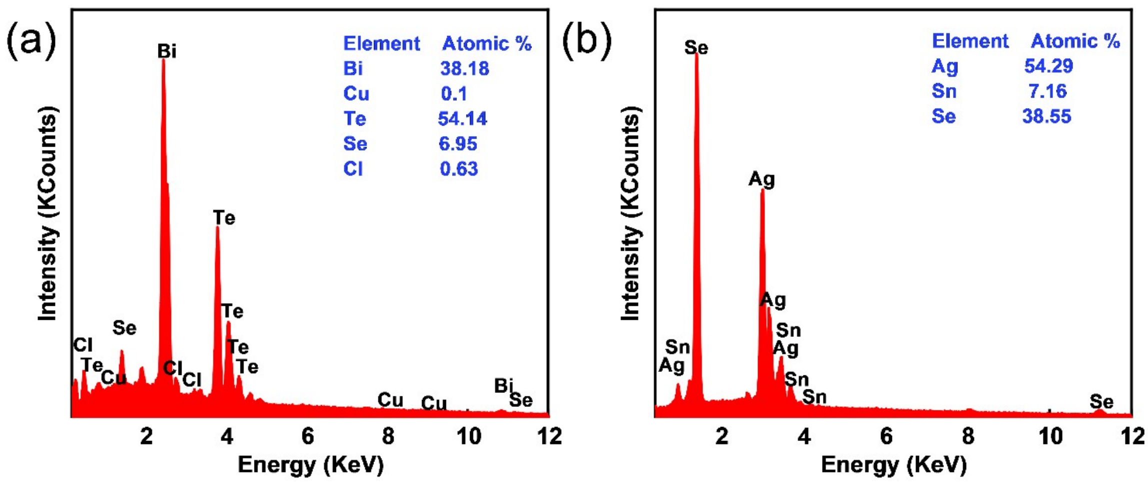

Figure. S2. The energy dispersive spectrum (a) $Bi_{1.995}Cu_{0.005}Te_{2.69}Se_{0.33}Cl_{0.03}$; (b) x = 0.5 wt% STSe.

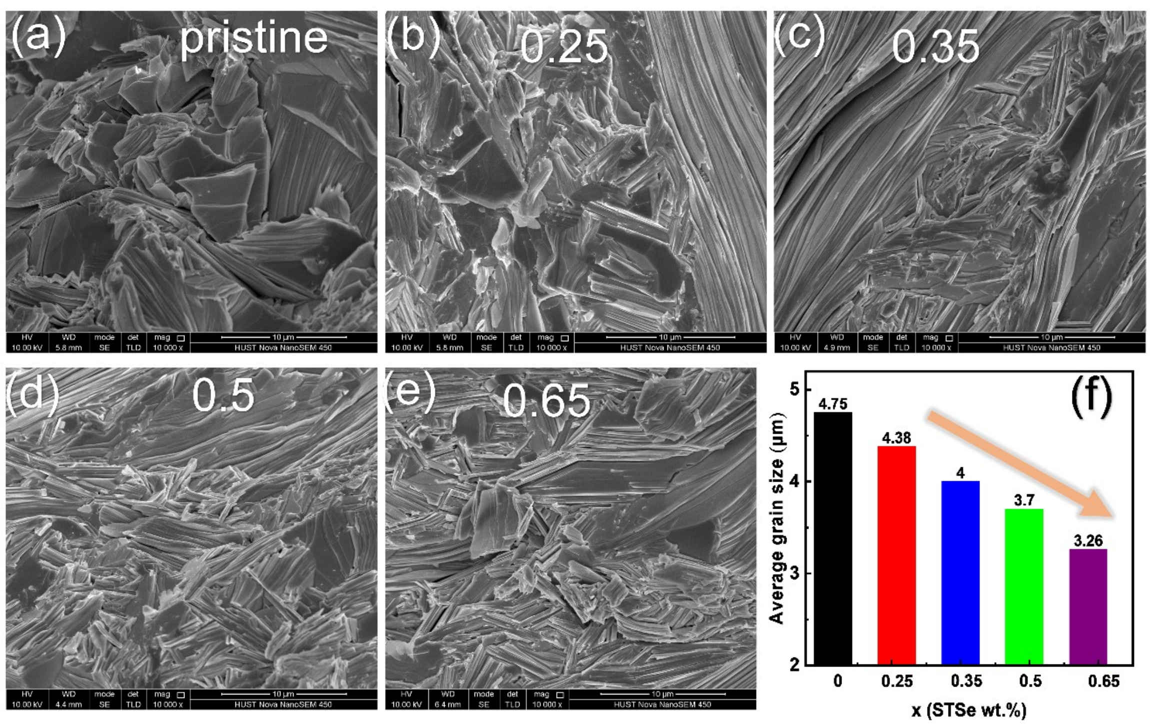

Figure S3 FSEM of fractured surface of (a) $Bi_{1.995}Cu_{0.005}Te_{2.69}Se_{0.33}Cl_{0.03}$; and (b-e) STSe wt%. (f) average grain size of all the samples.

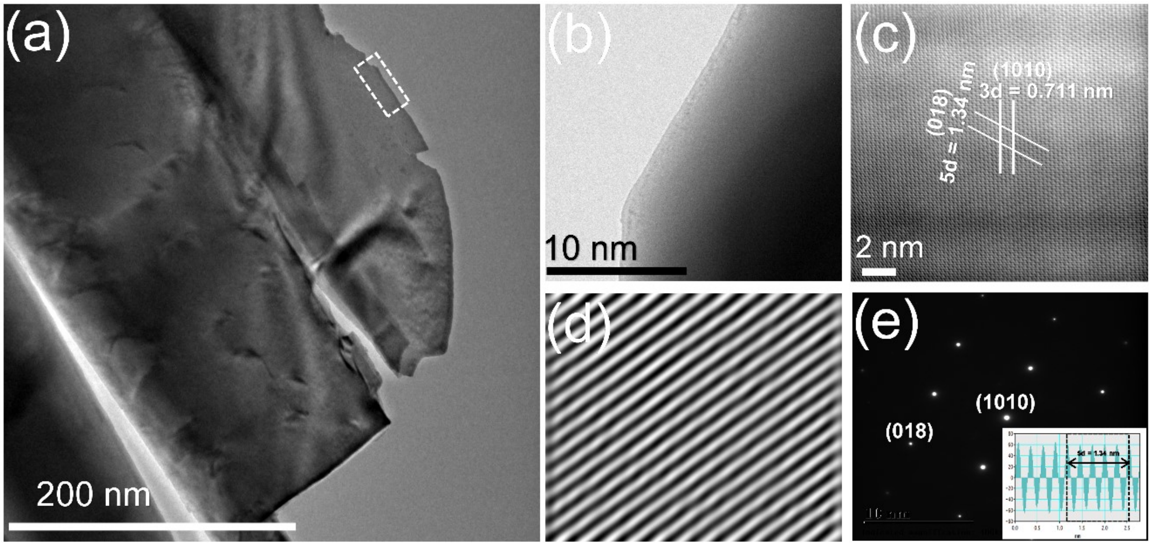

Figure S4. Characterization of Nanostructures in $Bi_{1.995}Cu_{0.005}Te_{2.69}Se_{0.33}Cl_{0.03}$: (a) Low-magnification TEM (LM-TEM) image; (b) Enlarged LM-TEM image of the area highlighted with a white-dashed rectangle; (c) Corresponding HR-TEM image of (a) exhibiting various interplanar spacings, and (d) Inverse Fast Fourier Transform (IFFT) (e) Selected area diffraction with inset d intensity profile of (c).

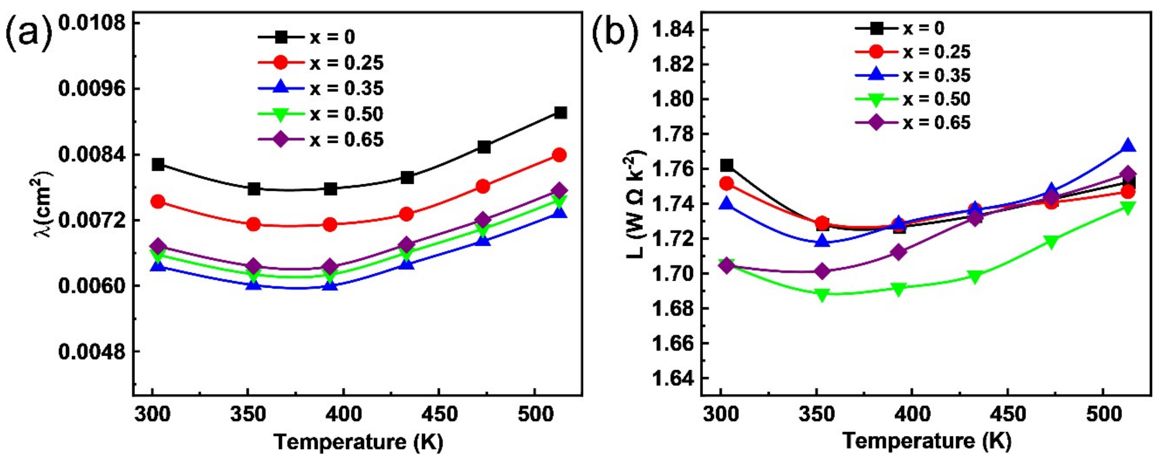

Figure. S5. (a) Thermal diffusivity; (b) Lorentz constant; (d) $Bi_{1.995}Cu_{0.005}Te_{2.69}Se_{0.33}Cl_{0.03}$ + *x* wt% STSe.

The estimation of specific heat[1]

$$C_P = C_v + (CTE)^{2T}/\beta_T D \qquad S4$$

$$C_v = 9nR\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx \qquad S5$$

$$C_v/3nR = D(T,\theta_D,n) = 1 + d_1(\theta_D/T) + d_2(\theta_D/T)^2 + \cdots + d_9(\theta_D/T)^9 \qquad S6$$

$$C_P \approx C_v + AC_P^2 T \qquad S7$$

where CTE is the coefficient of thermal expansion, β_T is the isothermal compressibility, D is the density, θ_D is the Debye temperature, R is the universal gas constant. At low temperatures (T<< θ_D), the Debye T^3 law, and it becomes the Dulong-Petit limit of 3R at T >> θ_D. Cv/3R is the Debye function and n is atoms per unit formula.

The equations for SPB model are:

$$m^* = \frac{h^2}{2k_B T}\left[\frac{n}{4\pi F_{\frac{1}{2}}(\eta)}\right]^{2/3} \qquad S8$$

The Seebeck coefficients, the scattering factor r = -1/2 in acoustic phonon scattering

$$S = -\frac{k_B}{e}\left(\frac{\left(r + \frac{3}{2}\right)F_{r+\frac{3}{2}}(\eta)}{\left(r + \frac{3}{2}\right)F_{r+\frac{1}{2}}(\eta)} - \eta\right) \qquad S9$$

The integral F_b η is defined by

$$F_b(\eta) = \int_0^{\infty} \frac{x^b}{1 + e^{x-\eta}} dx \qquad S10$$

$$\eta = -\frac{E_f}{k_B T} \qquad S11$$

Where F_b η is the Fermi integral function of order b, and η is the reduced Fermi energy.

The Lorenz number obtained based on the single parabolic band:

$$L = \left(\frac{k_B}{e}\right)^2 \left(\frac{\left(r+\frac{7}{2}\right)F_{r+\frac{5}{2}}(\eta)}{\left(r+\frac{3}{2}\right)F_{r+\frac{1}{2}}(\eta)} - \left[\frac{\left(r+\frac{5}{2}\right)F_{r+\frac{3}{2}}(\eta)}{\left(r+\frac{3}{2}\right)F_{r+\frac{1}{2}}(\eta)}\right]^2 \right) \qquad S12$$

Reference

(1) Wang, H., Porter, W.D., Böttner, H., König, J., Chen, L., Bai, S., Tritt, T.M., Mayolet, A., Senawiratne, J., Smith, C. and Harris, F. Transport properties of bulk thermoelectrics: an international round-robin study, part II: thermal diffusivity, specific heat, and thermal conductivity. *Journal of electronic materials 2013, 42,1073-1084*.