Electronic Supporting Information (ESI)

The origin of low thermal conductivity in $Sn_{1-x}Sb_xTe$: phonon scattering via layered intergrowth nanostructures

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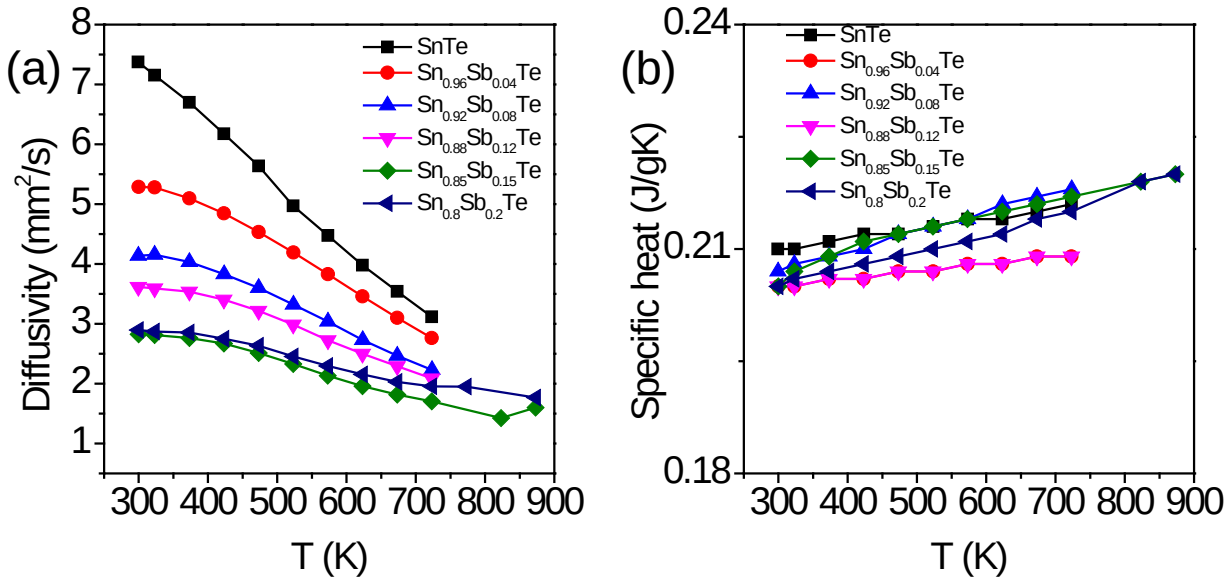


Figure S1. (a) Temperature dependent diffusivity (D) of $Sn_{1-x}Sb_xTe$. (b) Temperature dependent heat capacity (C_p) of $Sn_{1-x}Sb_xTe$.

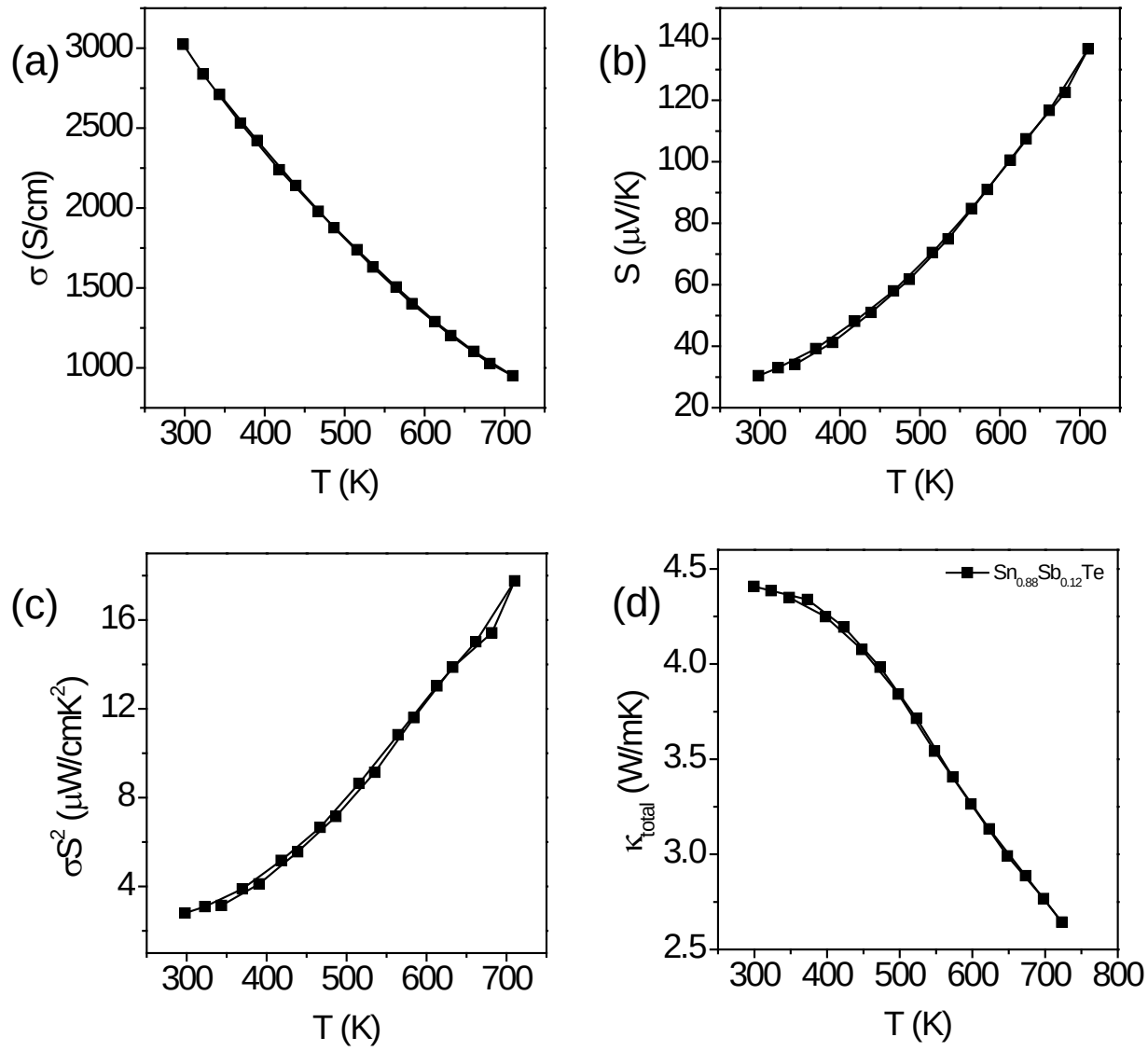


Figure S2. Heating and cooling cycle (a) electrical conductivity (σ), (b) Seebeck coefficient (S), (c) power factor (σS^2) and (d) thermal conductivity (κ_{total}) data of $Sn_{0.88}Sb_{0.12}Te$.

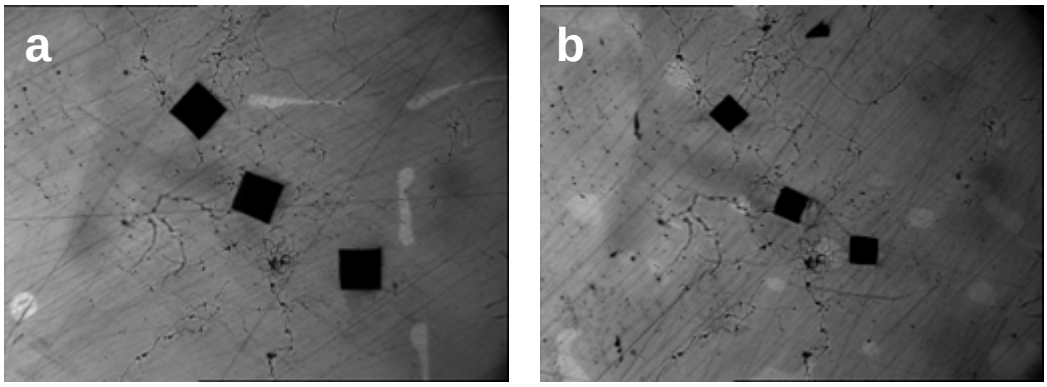


Figure S3. Vickers micro indentation of (a) SnTe and (b) $Sn_{0.85}Sb_{0.15}Te$, respectively.

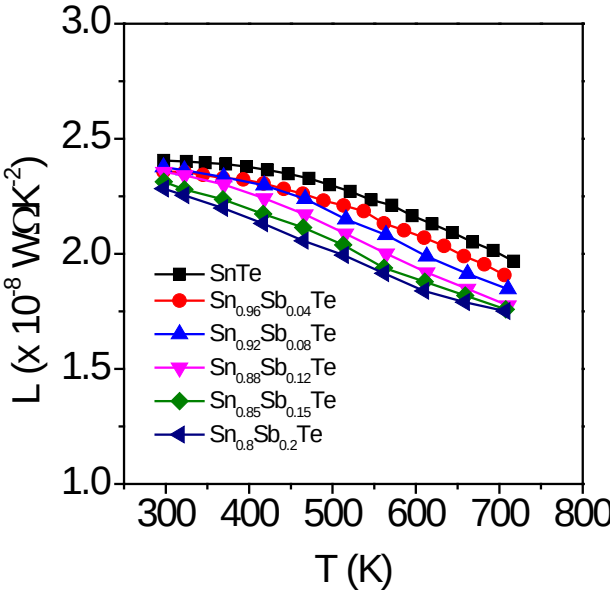


Figure S4. Temperature dependent Lorenz number (L) of $Sn_{1-x}Sb_xTe$.

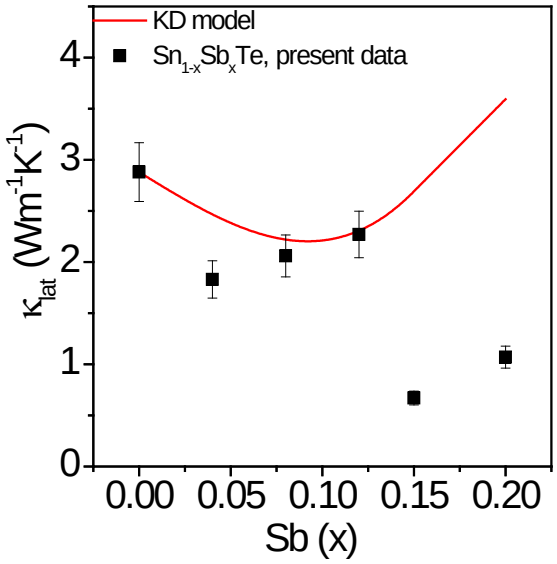


Figure S5. Room-temperature lattice thermal conductivity as a function of Sb alloying fraction x for $Sn_{1-x}Sb_xTe$, 10% error bars are indicated. The solid line is a solid solution line predicted by the Klemens–Drabble (KD) model.

Estimation of κ_{lat} of $Sn_{1-x}Sb_xTe$ from KD model:

According to Klemens–Drabble (KD) theory of disordered alloys, the lattice thermal conductivity of a disordered alloy, κ_{lat}^{d} is determined by:

$$\kappa_{lat}^{d} = \frac{\tan^{-1}(u)}{u}\,\kappa_{lat}^{p} \tag{1}$$

Where κ_{lat}^{p} is the lattice thermal conductivity of a pure alloy and u can be expressed by

$$u^2 = \frac{\pi^2 \Theta_D \Omega}{h v^2}\,\kappa_{lat}^{p}\Gamma \tag{2}$$

Here u is the disorder scaling parameter, Θ_D is the Debye temperature (Θ_D = 140 K for SnTe), h is the Plank constant, v is the sound velocity (v = 1800 m s^{-1}, for SnTe), and Ω is the volume per atom and Γ is the scattering parameter that combines the influences from mass, bonding force, and strain contrasts, described as

$$\Gamma = x(1-x)[\left(\frac{\Delta M}{M}\right)^2 + \varepsilon\,(\frac{\Delta a}{xa})^2] \tag{3}$$

where ε is a phenomenological parameter (163) related to the Grüneisen parameter γ (~2.1 for SnTe), M and a are the molar mass and lattice constant of the alloy, ΔM and Δa are the differences in mass and lattice constant between the two constituents.

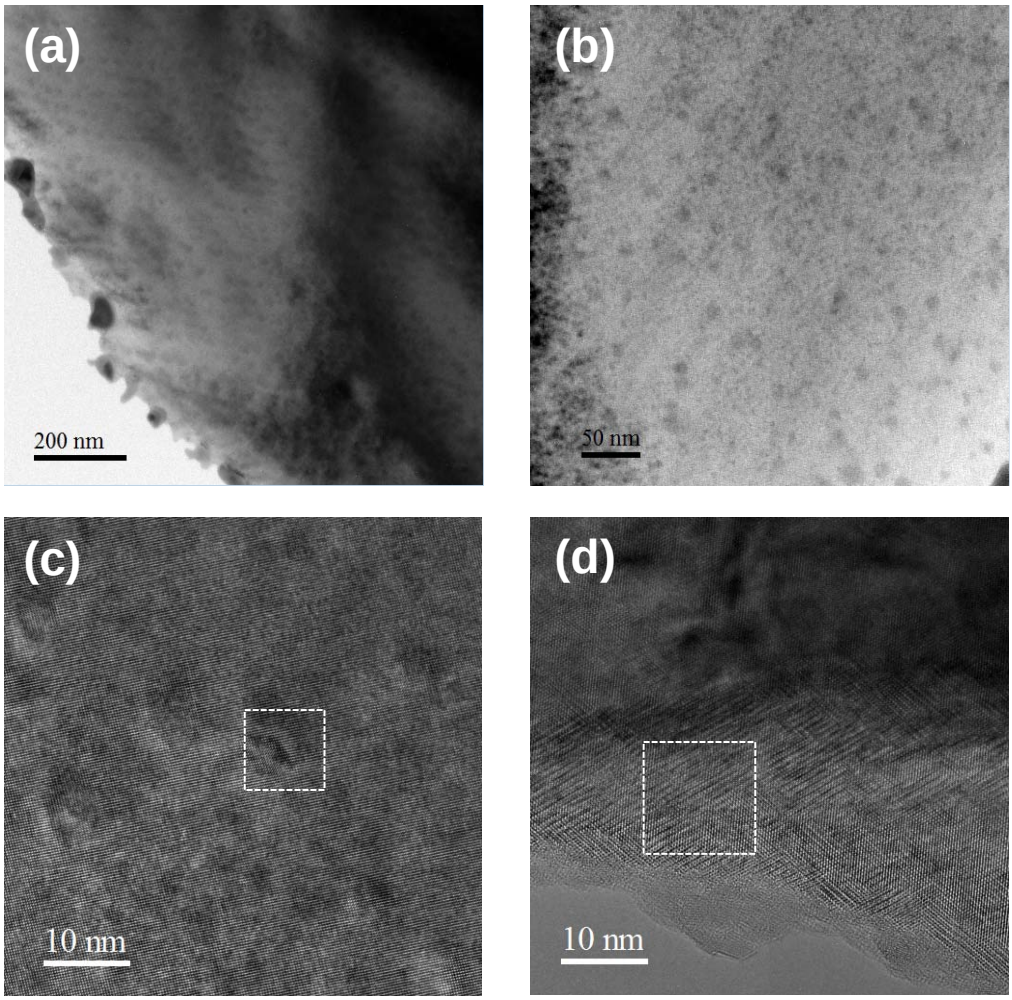
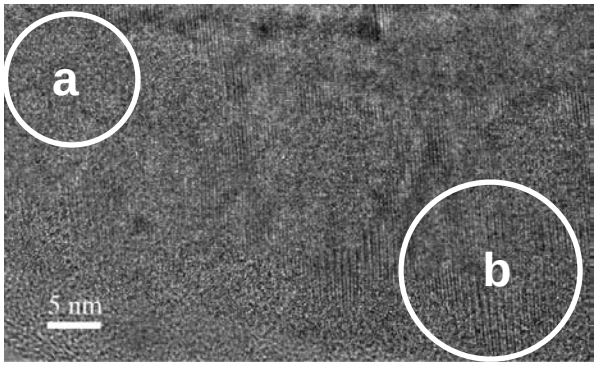


Figure S6. Low-magnification TEM images of the samples show nanoscale precipitates of $Sn_{0.92}Sb_{0.08}Te$ and $Sn_{0.85}Sb_{0.15}Te$ respectively in (a) and (b). (c) The HRTEM images of nanoscale precipitates of $Sn_{0.96}Sb_{0.04}Te$. (d) HRTEM image of $Sn_{0.85}Sb_{0.15}Te$ showing the presence of layered intergrowth nanodomains.



Spots	Atomic % of Sb	Atomic % of Sn	Atomic % of Te
a	2.3	38.7	58.82
b	13	49.80	38.42

Figure S7. HRTEM image of $Sn_{0.85}Sb_{0.15}Te$ sample shows nanoscale domains highlighted by circles (a) and (b). Table showing presence of Sb rich phase in layered nanostructured domain of sample.

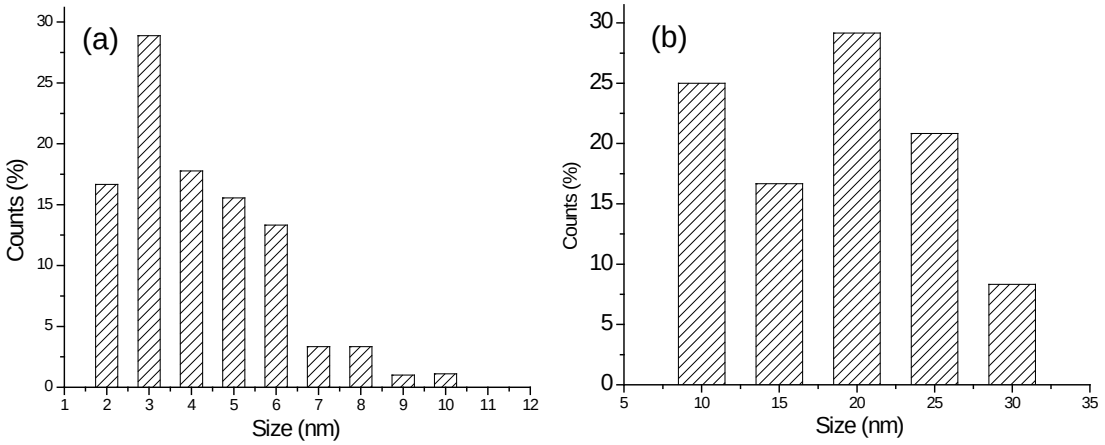


Figure S8. Size distribution histogram of the (a) nanoprecipitates in $Sn_{0.96}Sb_{0.04}Te$ and (b) intergrowth nanodomains in $Sn_{0.85}Sb_{0.15}Te$ samples.

Estimation of κ_{min} of SnTe: Theoretical limit for the minimum lattice thermal conductivity (κ_{min}) of SnTe was calculated based on the model proposed based on Cahil et al (Phys. Rev. B, 1992, 46, 6131–6140).

$$\kappa_{min} = \frac{3}{2}\left(\frac{\pi}{6}\right)^{\frac{1}{3}} k_B V^{-\left(\frac{2}{3}\right)} v$$

where, V is the unit cell volume, k_B is the Boltzman constant and v is the sound velocity (~1800 m/s) for SnTe.