Supporting information

Enhanced thermoelectric performance of In-doped and AgCuTe-alloyed SnTe through band engineering and endotaxial nanostructures

*Panpan Peng,[a] Chao Wang,[*a] Lanwei Li,[a] Shuyao Li,[a] Jing Chen,[*b] Pengya Fan,[a] Rui Du,[a] Haotian Si,[a] Zhenxiang Cheng[c] and Jianli Wang[*a,c]*

[a] *Institute for Computational Materials Science, School of Physics and Electronics, Henan University, Kaifeng, 475004, China; E-mail: wangchao@vip.henu.edu.cn*

[b] *Department of Technology and Physics, Zhengzhou University of Light Industry, Zhengzhou, 450002, China; E-mail: wulicj@126.com*

[c] *Institute for Superconducting and Electronic Materials, Innovation Campus, University of Wollongong, Squires Way, North Wollongong, Australia; E-mail: jianli@uow.edu.au*

Results and Discussion:

In our work, the Lorenz number is obtained based on the two band model:

$$L_{1h} = \left(\frac{\kappa_B}{e}\right)^2 \left[\frac{{}^2F_{-2}^1(\eta,\alpha)}{{}^0F_{-2}^1(\eta,\alpha)} - \left(\frac{{}^1F_{-2}^1(\eta,\alpha)}{{}^0F_{-2}^1(\eta,\alpha)}\right)^2\right], \quad (1)$$

and

$$L_{hh} = \left(\frac{\kappa_B}{e}\right)^2 \left[\frac{{}^2F_{-2}^1(\eta-\Delta\nu,0)}{{}^0F_{-2}^1(\eta-\Delta\nu,0)} - \left(\frac{{}^1F_{-2}^1(\eta-\Delta\nu,0)}{{}^0F_{-2}^1(\eta-\Delta\nu,0)}\right)^2\right], \quad (2)$$

In the equations above the integral ${}^nF_l^m$ is defined by

$${}^nF_l^m = \int_0^\infty -\frac{\partial f}{\partial \varepsilon}\varepsilon^n\left(\varepsilon+\alpha\varepsilon^2\right)^m\left[\left(1+2\alpha\varepsilon\right)^2+2\right]^{\frac{l}{2}} d\varepsilon,$$

where L_{lh} is the L of light-hole band, L_{hh} is the L of heavy-hole band, η is the reduced

chemical potential calculated by $\eta = {}^{E_f}/_{k_B T}$, α is the nonparabolic parameter obtained by $\alpha = {}^{k_B T}/_{E_g}$, and ${}^{n}F_l^m$ is the generalized Fermi function. For the second valence band, we set α = 0 and replace η with η-Δv in these equations, where $\Delta v = {}^{\Delta E}/_{k_B T}$, Δ$E$ is the energy difference between the first and second valence band. The total L of the system can be expressed:

$$L_{total} = \left(\delta_{1h} L_{1h} + \delta_{hh} L_{hh}\right) / \left(\delta_{1h} + \delta_{hh}\right).$$

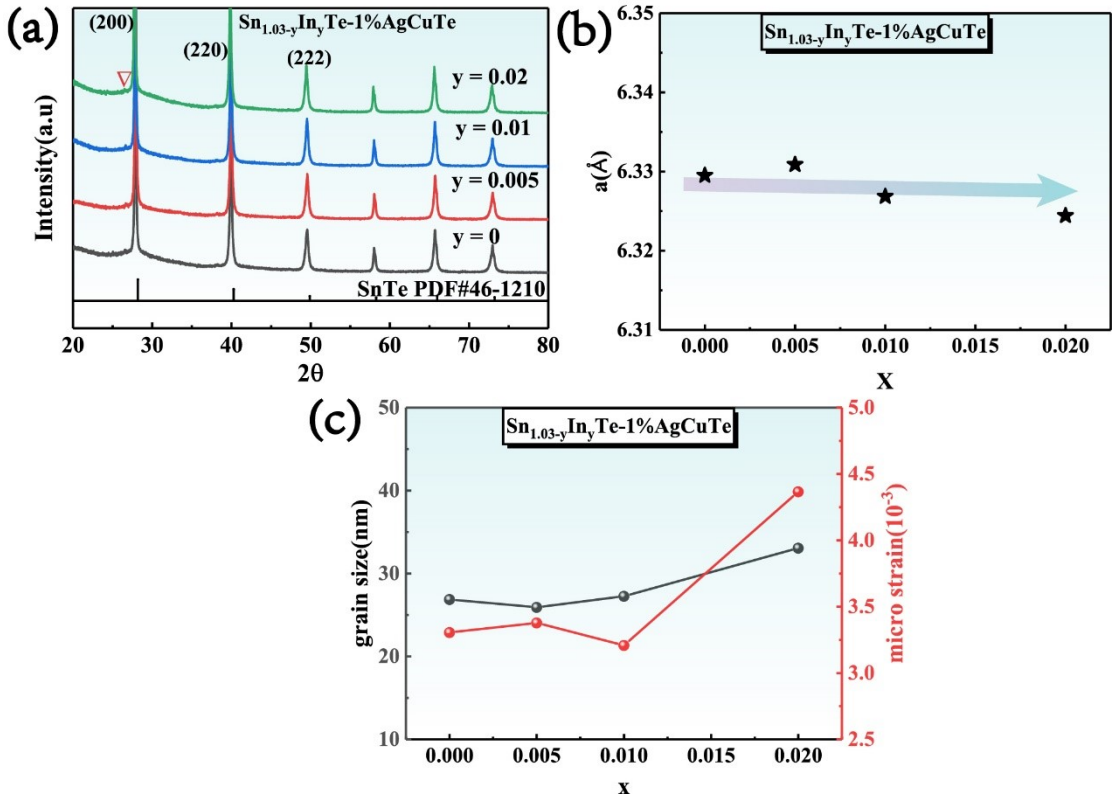

Figure S1 (a) XRD patterns, (b) lattice parametes (c) average grain size and micro strain of Sn $_{1.03-y}$ In $_y$ Te-x%AgCuTe.

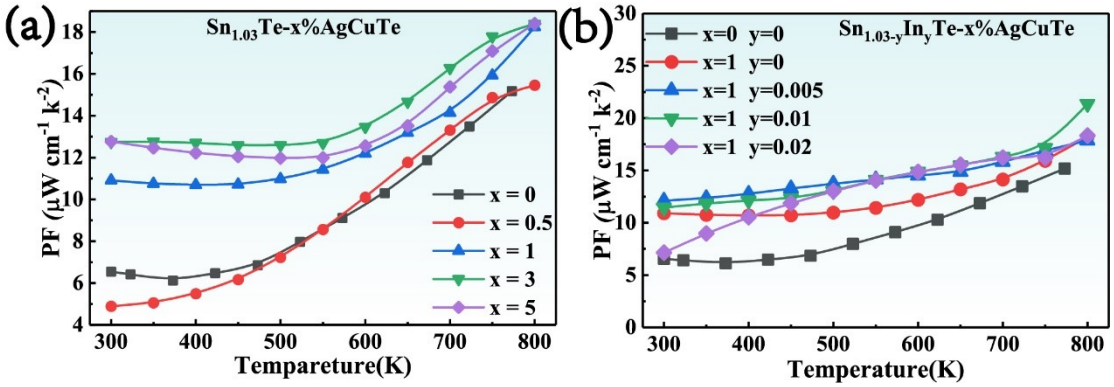

Figure S2. (a), (b) power factors as the function of temperature for $Sn_{1.03}Te$-x%AgCuTe and $Sn_{1.03-y}In_yTe$-1%AgCuTe, respectively.

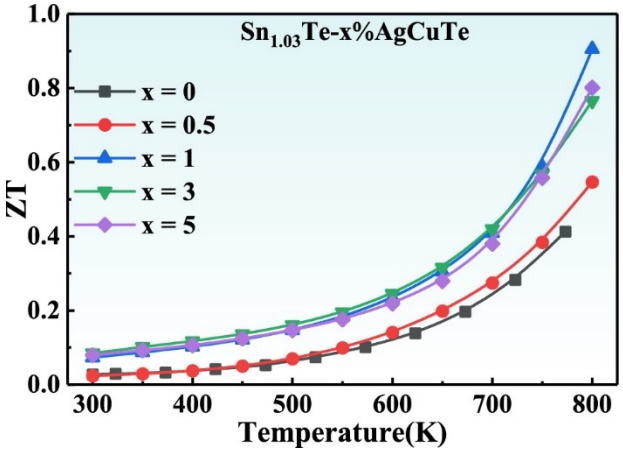

Figure S3. ZT values as the function of temperature for $Sn_{1.03}Te$-x%AgCuTe.

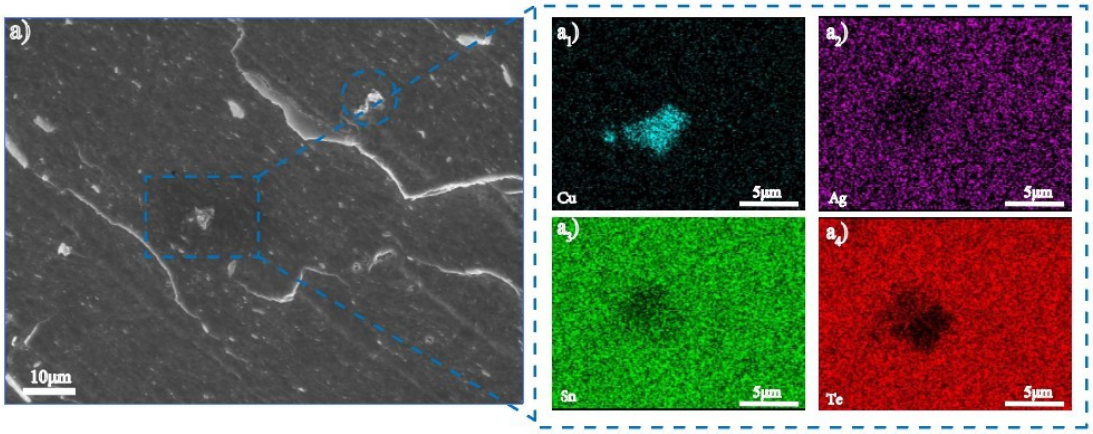

Figure S4. (a) SEM images of $Sn_{1.03}Te$-5%AgCuTe sample. (a1)-(a4) Elemental energy dispersive spectroscopy (EDS) mapping of the $Sn_{1.03}Te$-5%AgCuTe sample.

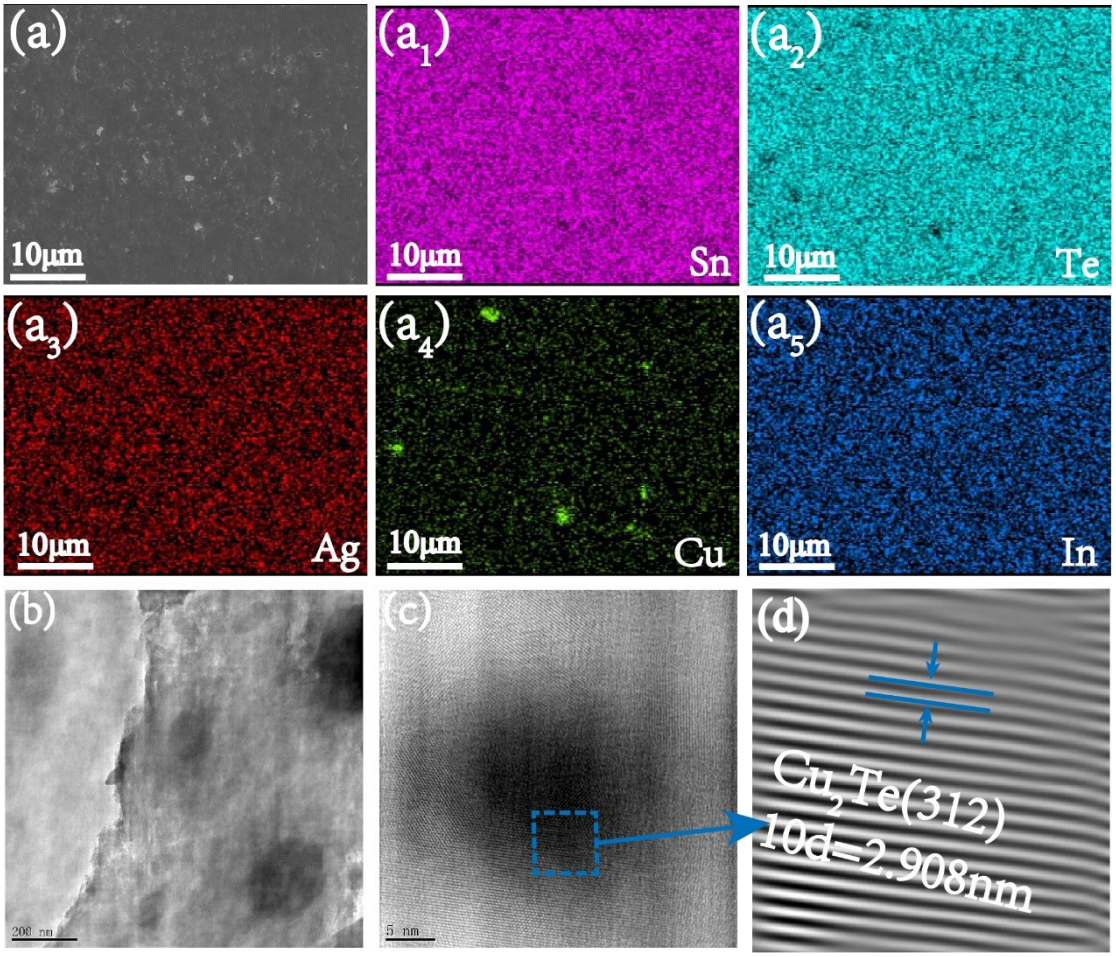

Figure S5 (a) SEM images of $Sn_{1.01}In_{0.02}$ Te-1%AgCuTe sample. (a1-a5) Elemental energy dispersive spectroscopy (EDS) mapping of the $Sn_{1.01}In_{0.02}$Te-1%AgCuTe sample. (b) TEM image of the $Sn_{1.02}In_{0.01}$Te-1%AgCuTe. (c) HRTEM image of $Sn_{1.02}In_{0.01}$Te-1%AgCuTe; (d) the IFFT image of the blue rectangle in plot (c)