Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Contrasting roles of Bi- doping and Bi_2Te_3 alloying on the thermoelectric performance of SnTe

Fudong Zhang[a,#], Xia Qi[a,#], Mingkai He[b], Fengshan Zheng[c], Lei Jin[c,*], Zhanhui Peng[a], Xiaolian Chao[a], Zupei Yang[a,*], Di, Wu[a,*]

[a] Key Laboratory for Macromolecular Science of Shaanxi Province, School of Materials Science and Engineering, Shaanxi Normal University, Xi'an 710062, China.

[b] Department of Physics, The Chinese University of Hong Kong, Hong Kong 999077, China

[c] Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons Forschungszentrum Jülich GmbH 52428 Jülich, Germany.

[#] These authors contributed equally to this work.

*Correspondence shall be addressed to:

E-mails: l.jin@fz-juelich.de, yangzp@snnu.edu.cn, wud@snnu.edu.cn.

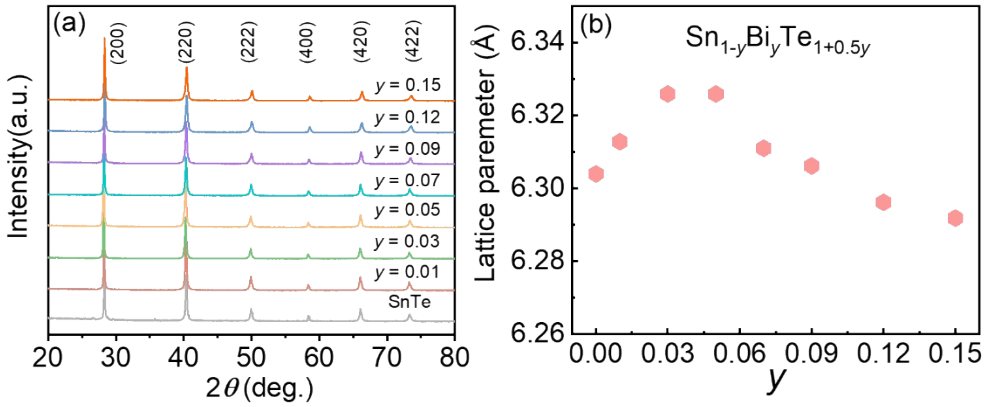

Figure S1 (a) The powder XRD patterns for $Sn_{1-y}Bi_yTe_{1+0.5y}$ (y = 0, 0.01, 0.03, 0.05, 0.07, 0.09, 0.12, 0.15). (b) Calculated lattice parameters obtained from (a).

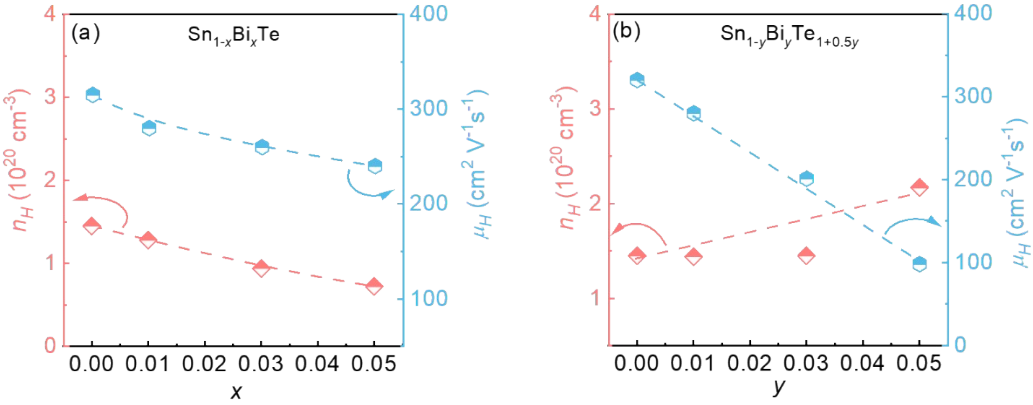

Figure S2 (a) and (b) Room-temperature carrier concentration (n_H) and carrier mobility (μ_H) of $Sn_{1-x}Bi_xTe$ and $Sn_{1-y}Bi_yTe_{1+0.5y}$, respectively.

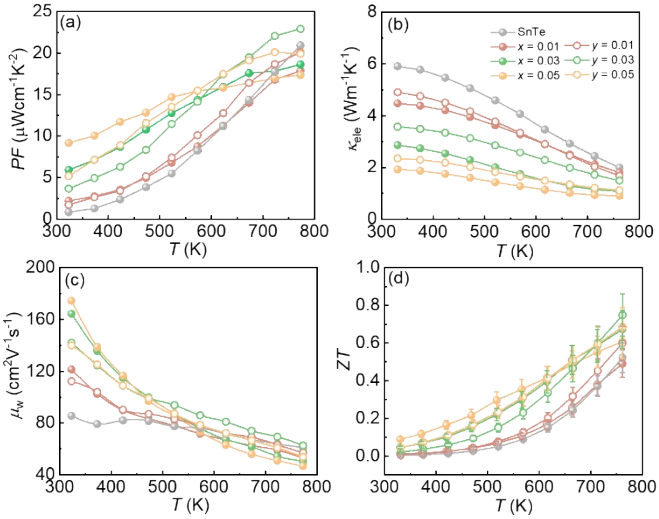

Figure S3 Temperature dependent (a) power factor, (b) calculated electronic thermal conductivity, (c) calculated weighted carrier mobility, and (d) *ZT* of $Sn_{1-x}Bi_xTe$ (x = 0, 0.01, 0.03 and 0.05) and $Sn_{1-y}Bi_yTe_{1+0.5y}$ (y = 0, 0.01, 0.03 and 0.05).

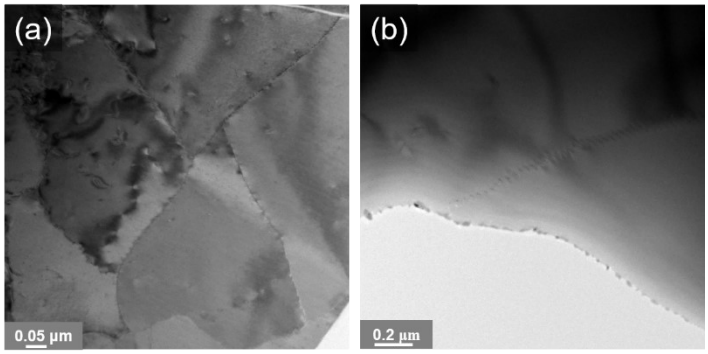

Figure S4 Low magnification TEM image of $Sn_{0.97}Bi_{0.03}Te_{1.015}$ sample showing (a) mesoscale grains and (b) dislocation arrays at grain boundaries.

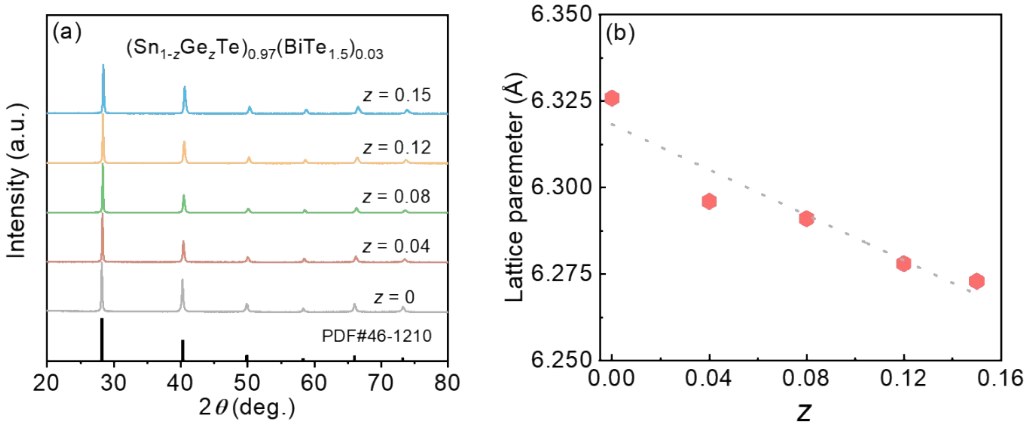

Figure S5 (a) The powder X-ray diffraction (XRD) patterns and (b) calculated lattice parameters of $(Sn_{1-z}Ge_zTe)_{0.97}$-$(BiTe_{1.5})_{0.03}$ (z = 0, 0.04, 0.08, 0.12 and 0.15).

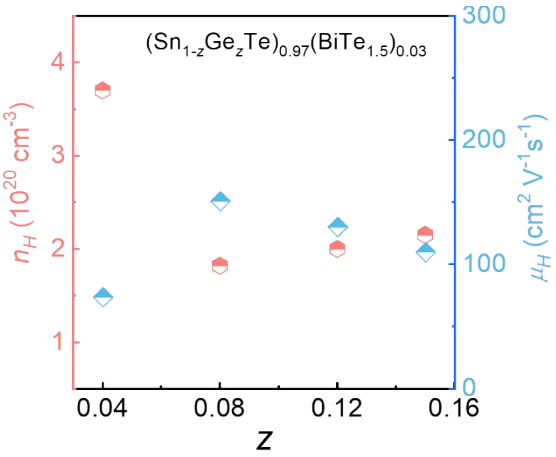

Figure S6 Room-temperature carrier concentration (n_H) and carrier mobility (μ_H) of $(Sn_{1-z}Ge_zTe)_{0.97}$-$(BiTe_{1.5})_{0.03}$ (z = 0.04, 0.08, 0.12 and 0.15).