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

Supporting Information

Multiple effect of Bi doping to enhanced thermoelectric properties of SnTe

Zhiwei Zhou, Junyou Yang, Qinghui Jiang, Yubo Luo, Dan Zhang, Yangyang Ren, Xu He, Jiwu Xin*

State Key Laboratory of Materials Processing and Die & Mould Technology, Huazhong University of Science and Technology, Wuhan 430074, P. R China

* To whom correspondence should be addressed. Email: jyyang@mail.hust.edu.cn

1. Rietveld refinements

The PXRD patterns of $Sn_{1-x}Bi_xTe$ (x=0, 0.02 0.04 0.06 0.08) have been refined by the GSAS with EXPGUI interface.[27-28]

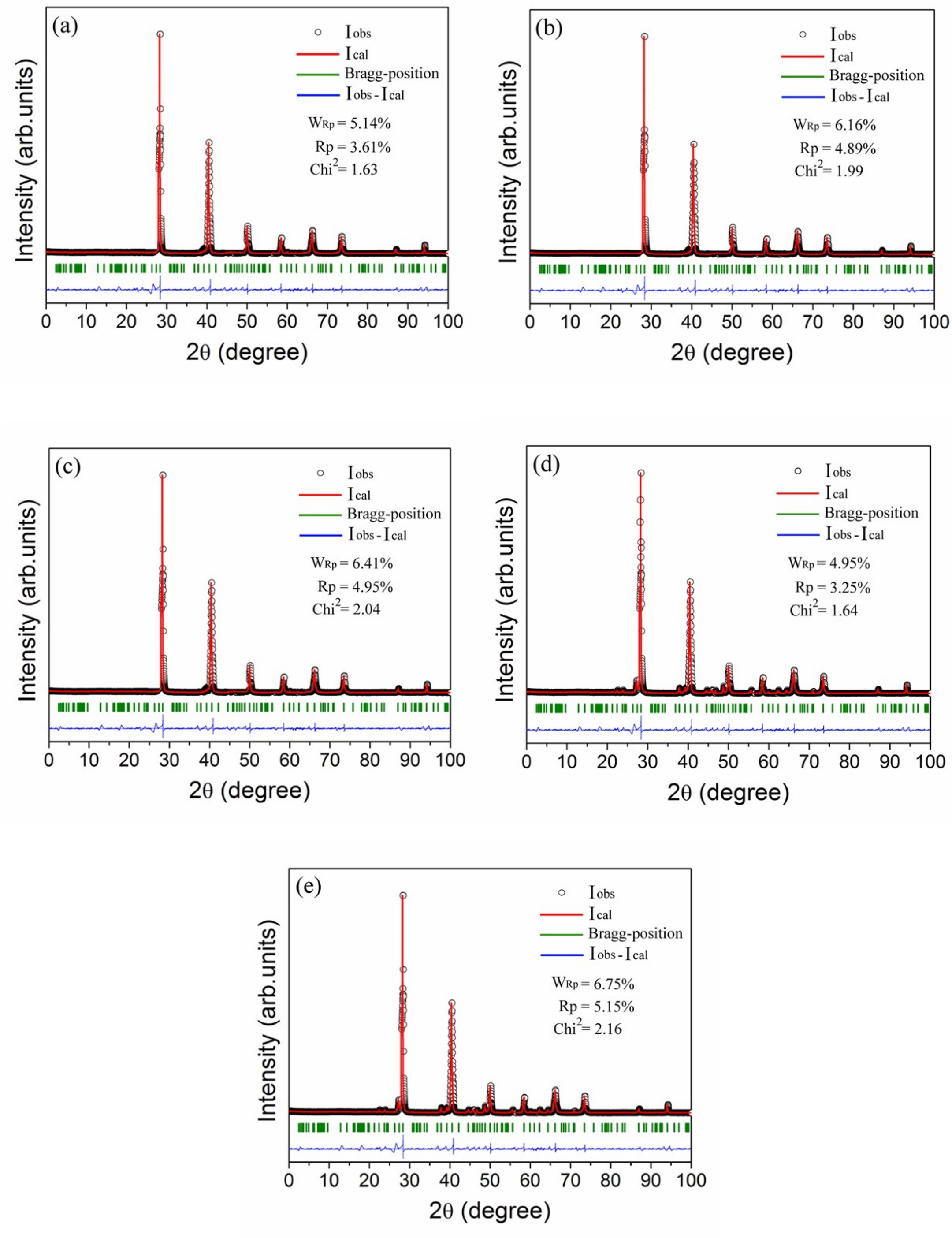

Fig. S1 Rietveld refinements of $Sn_{1-x}Bi_xTe$ (x=0, 0.02, 0.04, 0.06, 0.08).

2. Elemental mapping

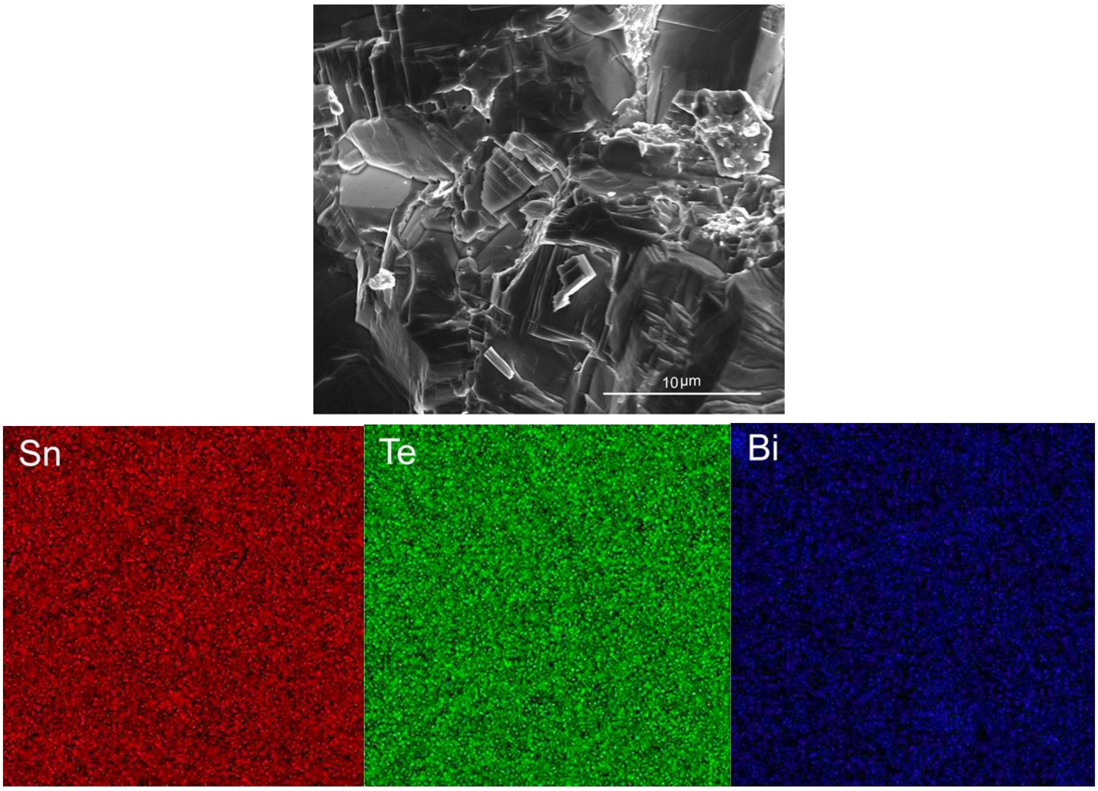

Fig. S2 The elemental mapping of $Sn_{0.94}Bi_{0.06}Te$.

3. Specific heat capacity (C_P)

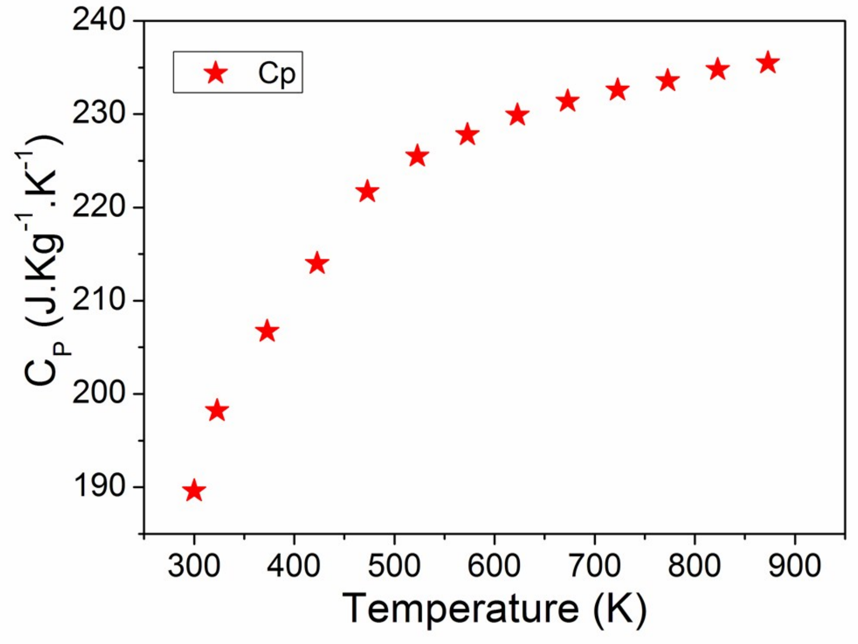

Fig. S3 The temperature dependence of the specific heat capacity.[24]

4. The test of reversibility and recyclability

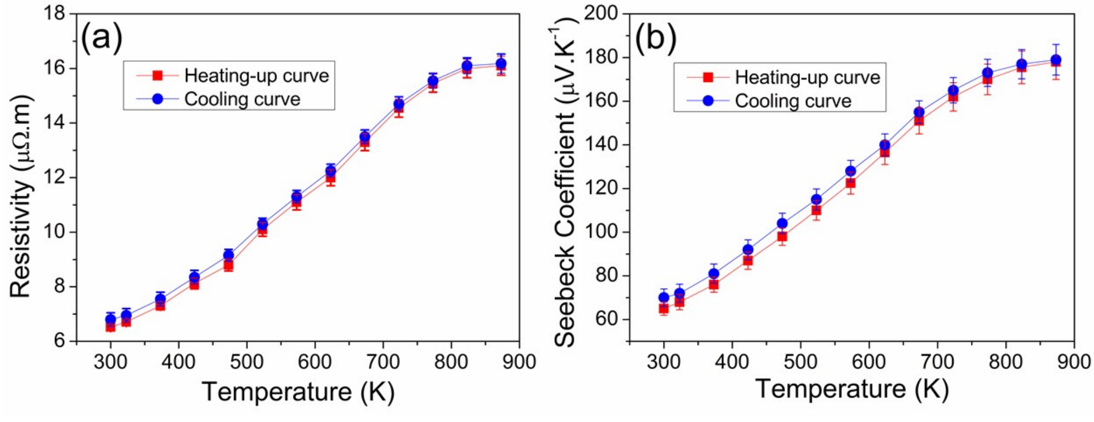

Fig. S4 The test of reversibility for the sample of $Sn_{0.94}Bi_{0.06}Te$.

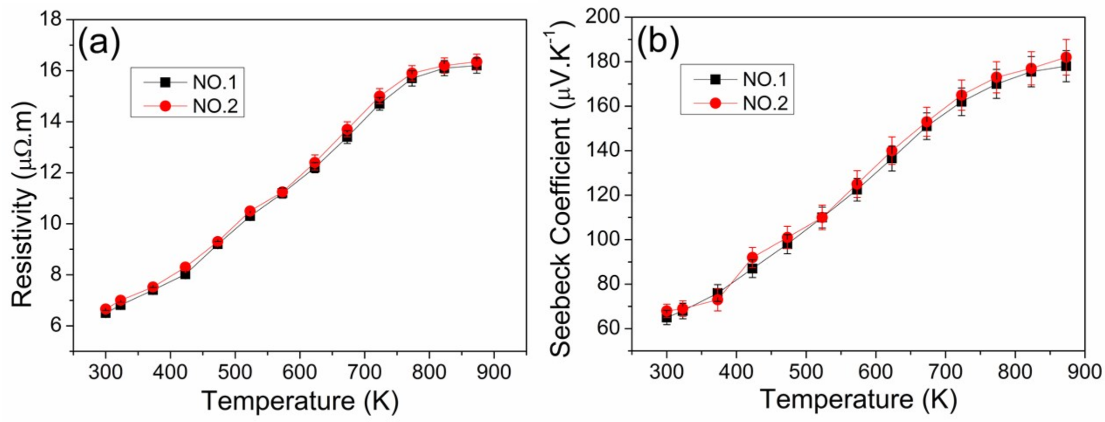

Fig. S5 The test of recyclability for the sample of $Sn_{0.94}Bi_{0.06}Te$.

5. Pisarenko line

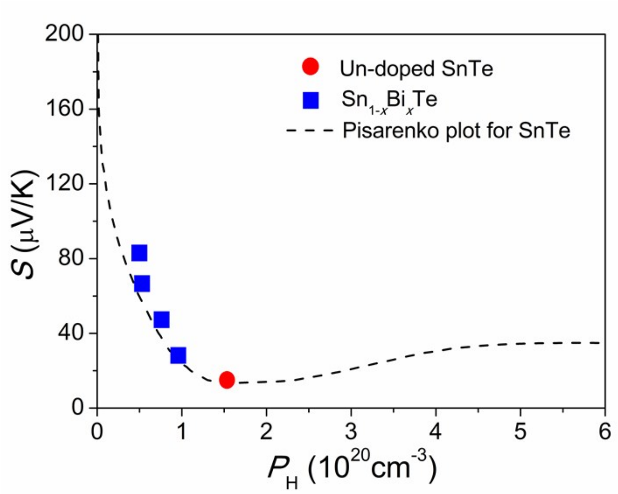

Figure S6. Room temperature Seebeck coefficient as a function of hole density for Bi doped SnTe. The dotted line is Pisarenko plot expected by a VBM model.

Table S1. Parameters of all the samples investigated in this study.

Samples	Effective mass m* (m_0)	Densities (g/cm^3)	Relative densities (%)	Lorenz number ($10^{-8}V^2/K^2$)
x=0	0.179	6.28	96.61	2.4307
x=0.02	0.336	6.27	96.46	2.3402
x= 0.04	0.391	6.29	96.77	2.2518
x= 0.06	0.49	6.32	97.23	2.1235
x= 0.08	0.634	6.34	97.53	1.9956

The effective mass (m*) is estimated according to the following equations using the observed carrier concentration (n_h) and Seebeck coefficient (S) values:

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

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

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

Here, η is the reduced Fermi energy, $F_n(\eta)$ is the nth order Fermi integral, κ_B is the Boltzmann constant, e is the electron charge, h is the Planck constant and r is the scattering factor.