补充材料 (2022 *Acta Phys. Sin.* **71** 237302)

Improvement of thermoelectric performance of SnTe-based solid solution by entropy engineering technology*

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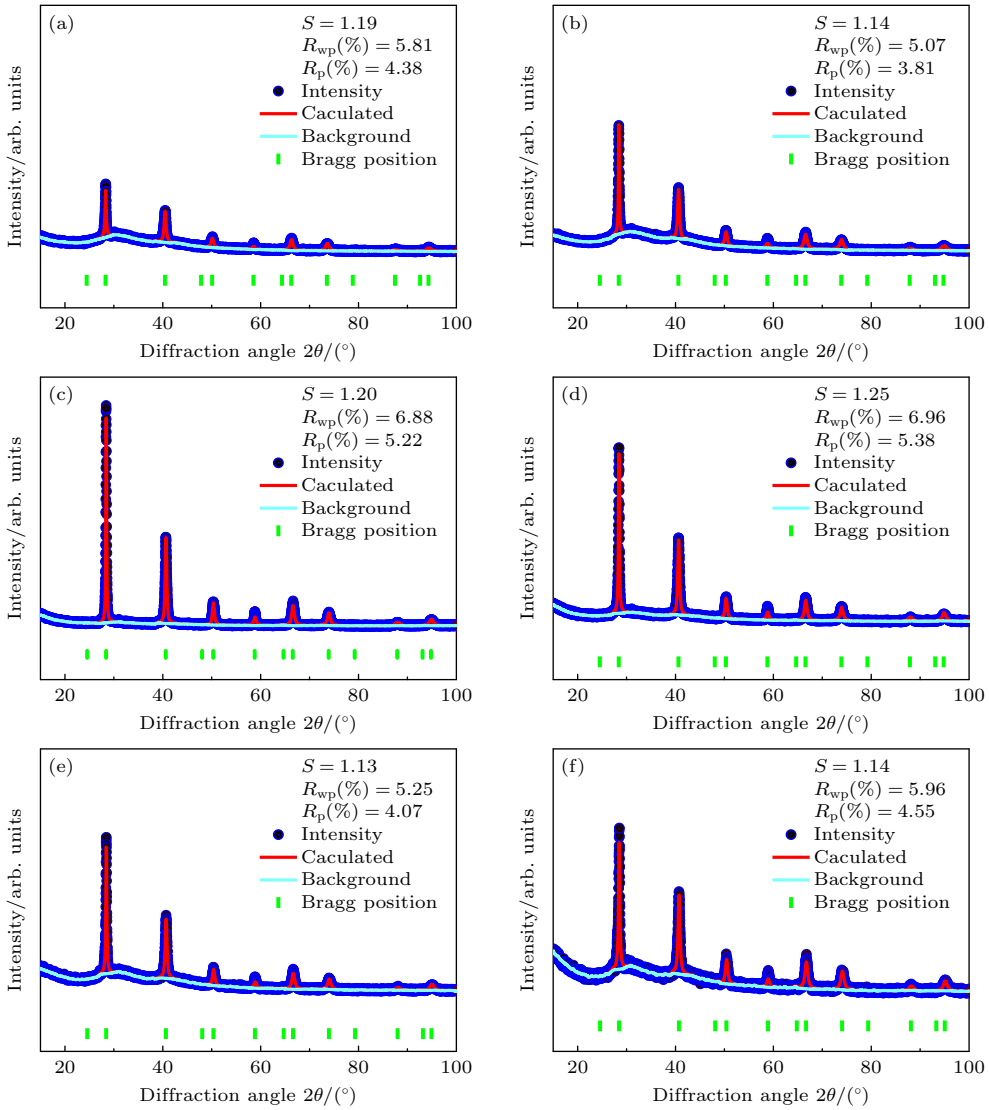

Fig. S1. XRD refinement patterns of different kinds of materials: (a) $Sn_{0.95}Ge_{0.05}Te$; (b) $(Sn_{0.95}Ge_{0.05}Te)_{0.95}(Ag_2Se)_{0.05}$; (c) $(Sn_{0.925}Ge_{0.05}Bi_{0.025}Te)_{0.95}(Ag_2Se)_{0.05}$; (d) $(Sn_{0.9}Ge_{0.05}Bi_{0.05}Te)_{0.95}(Ag_2Se)_{0.05}$; (e) $(Sn_{0.875}Ge_{0.05}Bi_{0.075}Te)_{0.95}(Ag_2Se)_{0.05}$; (f) $(Sn_{0.85}Ge_{0.05}Bi_{0.1}Te)_{0.95}(Ag_2Se)_{0.05}$.

* 国家自然科学基金 (批准号: 51671109) 资助的课题.

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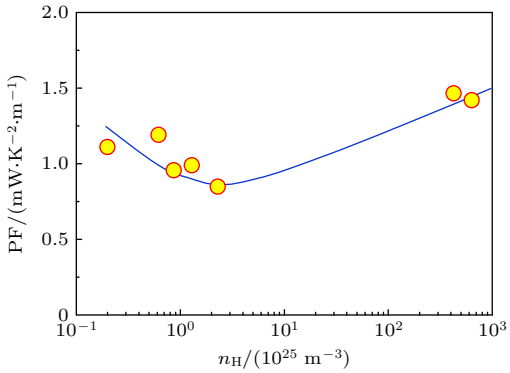

Fig. S2 Power factors (PF) versus Hall carrier concentration (n_H) at room temperature for samples of $(Sn_{0.95-x}Ge_{0.05}Bi_xTe)_{0.95}(Ag_2Se)_{0.05}$ (x=0, 0.025, 0.05 0.075, 0.1).

Table S1. XRD-refined related structural parameters and crystallographic data.

Compositions	$Sn_{0.95}Ge_{0.05}Te$	$x = 0$	$x = 0.025$	$x = 0.05$	$x = 0.075$	$x = 0.1$
Space group	*Fm-3m*	*Fm-3m*	*Fm-3m*	*Fm-3m*	*Fm-3m*	*Fm-3m*
Z	4	4	4	4	4	4
a/Å	6.3042	6.2806	6.2778	6.2779	6.2736	6.2668
V/Å^3	250.55	247.73	247.41	247.45	246.89	246.11
R_p/%	4.38	3.81	5.22	5.38	4.07	4.55
R_{wp}/%	5.81	5.07	6.88	6.96	5.25	5.96
GOF	1.19	1.14	1.20	1.25	1.13	1.14

Table S2. Atomic coordinates, atomic occupations and Wcykoff positions for different samples.

Compositions	Atom	Site	x	y	z	B_{iso}	Occupancy
$Sn_{0.95}Ge_{0.05}Te$	Sn1	4a	0	0	0	0.0012	0.95
	Ge1	4a	0	0	0	0.0012	0.05
	Te1	4b	1/2	1/2	1/2	0.0039	1
$x = 0$	Sn1	4a	0	0	0	0.0089	0.9025
	Ge1	4a	0	0	0	0.0026	0.0475
	Ag1	4a	0	0	0	0.0026	0.05
	Te1	4b	1/2	1/2	1/2	0.0092	0.95
	Se1	4b	1/2	1/2	1/2	0.0102	0.05
$x = 0.025$	Sn1	4a	0	0	0	0.0106	0.87875
	Ge1	4a	0	0	0	0.0031	0.0475
	Ag1	4a	0	0	0	0.0031	0.05
	Bi1	4a	0	0	0	0.0100	0.02375
	Te1	4b	1/2	1/2	1/2	0.0111	0.95
	Se1	4b	1/2	1/2	1/2	0.0124	0.05
$x = 0.05$	Sn1	4a	0	0	0	0.0054	0.855
	Ge1	4a	0	0	0	0.0037	0.0475
	Ag1	4a	0	0	0	0.0037	0.05
	Bi1	4a	0	0	0	0.0114	0.0475
	Te1	4b	1/2	1/2	1/2	0.0049	0.95
	Se1	4b	1/2	1/2	1/2	0.0142	0.05
$x = 0.075$	Sn1	4a	0	0	0	0.0032	0.83125
	Ge1	4a	0	0	0	0.0050	0.0475
	Ag1	4a	0	0	0	0.0049	0.05
	Bi1	4a	0	0	0	0.0131	0.07125
	Te1	4b	1/2	1/2	1/2	0.0028	0.95
	Se1	4b	1/2	1/2	1/2	0.0180	0.05
$x = 0.1$	Sn1	4a	0	0	0	0.0009	0.8075
	Ge1	4a	0	0	0	0.0062	0.0475
	Ag1	4a	0	0	0	0.0059	0.05
	Bi1	4a	0	0	0	0.0050	0.095
	Te1	4b	1/2	1/2	1/2	0.0008	0.95
	Se1	4b	1/2	1/2	1/2	0.0174	0.05