Supporting Information

Efficient Sc-doped $Mg_{3.05-x}Sc_xSbBi$ thermoelectrics near room temperature

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Table S1. Room-temperature Hall carrier concentration (n_H), Hall mobility (μ_H), deformation potential coefficient (E_{def}), density-of-state effective mass (m^*_{DOS}), inertial effective mass(m_I^*), bulk modulus B, shear modulus G, Debye temperature Θ_D (K), Poisson ratio (ε) and Grüneisen constant (γ), density (d) and relative density (%) for $Mg_{3.05-x}Sc_xSbBi$ and $Mg_{3.05-x}Sc_xSb_{1.5}Bi_{0.5}$.

	composition	$\lvert n_H \rvert$ ($10^{19}cm^{-3}$)	$\lvert \mu_H \rvert$ ($cm^2V^{-1}s^{-1}$)	E_{def} (eV)	m^*_{DOS} (m_e)	m_I^* (m_e)	B (GPa)	G (GPa)	θ_D (K)	ε	γ	d (gcm^{-3})	Relative Density (%)
$Mg_{3.05-x}Sc_xBiSb$	x=0.001	0.30	109	23.23	1.16	/	41.1	14.6	190	0.34	2.07	4.96	96
	x=0.0015	0.45	135	22.21	1.08	/	39.3	13.9	186	0.34	2.07	5.01	97
	x=0.003	1.6	137	20.73	1.10	0.26	40.9	14.4	190	0.34	2.07	5.02	97
	x=0.005	3.4	120	15.77	1.42	0.23	40.7	14.0	187	0.35	2.09	5.11	98
	x=0.009	4.9	100	24.07	1.04	0.17	40.5	14.6	191	0.34	2.04	4.96	96
	x=0.012	6.0	98	23.65	1.04	0.21	40.2	14.7	191	0.34	2.03	5.02	97
	x=0.015	5.4	92	23.53	1.06	0.18	40.9	14.2	188	0.34	2.08	5.05	98
	x=0.018	5.3	107	21.26	1.13	0.14	40.3	14.0	187	0.34	2.08	4.98	97
	x=0.020	5.3	106	20.05	1.19	0.15	40.5	13.9	186	0.35	2.09	4.98	97
	x=0.025	5.7	106	25.69	0.95	0.13	39.9	13.6	184	0.35	2.11	5.05	98
	x=0.030	4.9	101	17.34	1.27	0.17	46.6	16.7	199	0.34	2.05	5.02	97
$Mg_{3.05-x}Sc_xBi_{0.5}Sb_{1.5}$	x=0.015	5.0	74	27.34	1.10	0.17	42.8	14.5	201	0.35	2.11	4.51	98
	x=0.030	5.2	76	27.56	1.07	0.16	41.0	14.0	197	0.35	2.10	4.48	98

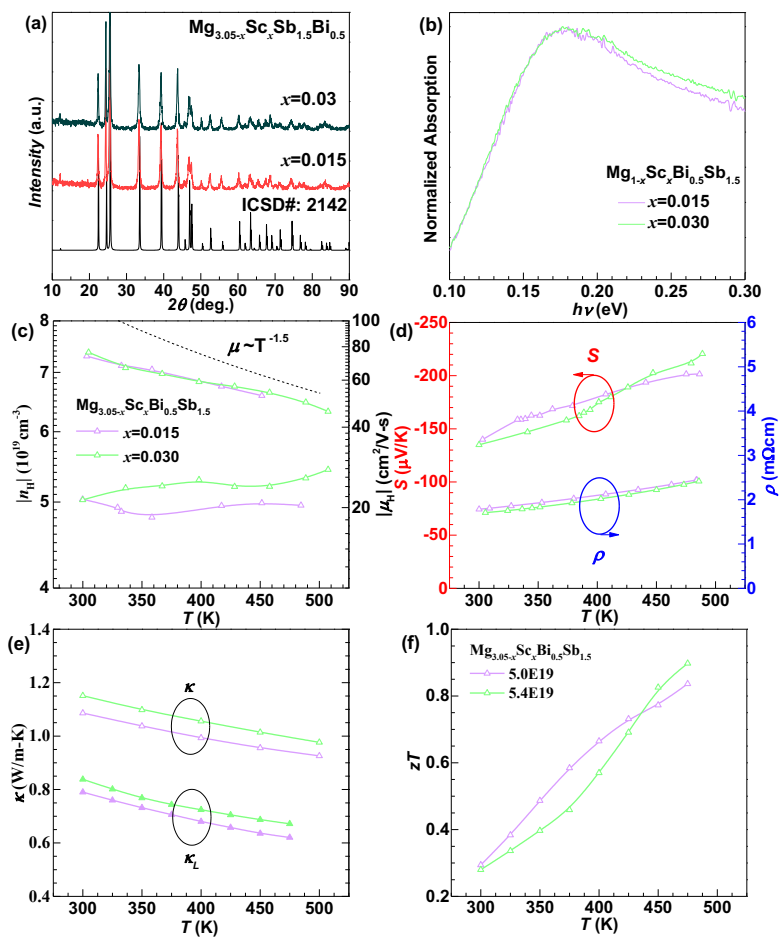

Fig. S1. (a) Room temperature powder XRD patterns for $Mg_{3.05-x}Sc_xBi_{0.5}Sb_{1.5}$ and (b) photon energy dependent normalized absorption, (c) temperature dependent Hall mobility (μ_H), (d) Hall carrier concentration (n_H), (c) Seebeck coefficient, (d) resistivity, (e) total thermal conductivity and (f) zT for $Mg_{3.05-x}Sc_xBi_{0.5}Sb_{1.5}$.

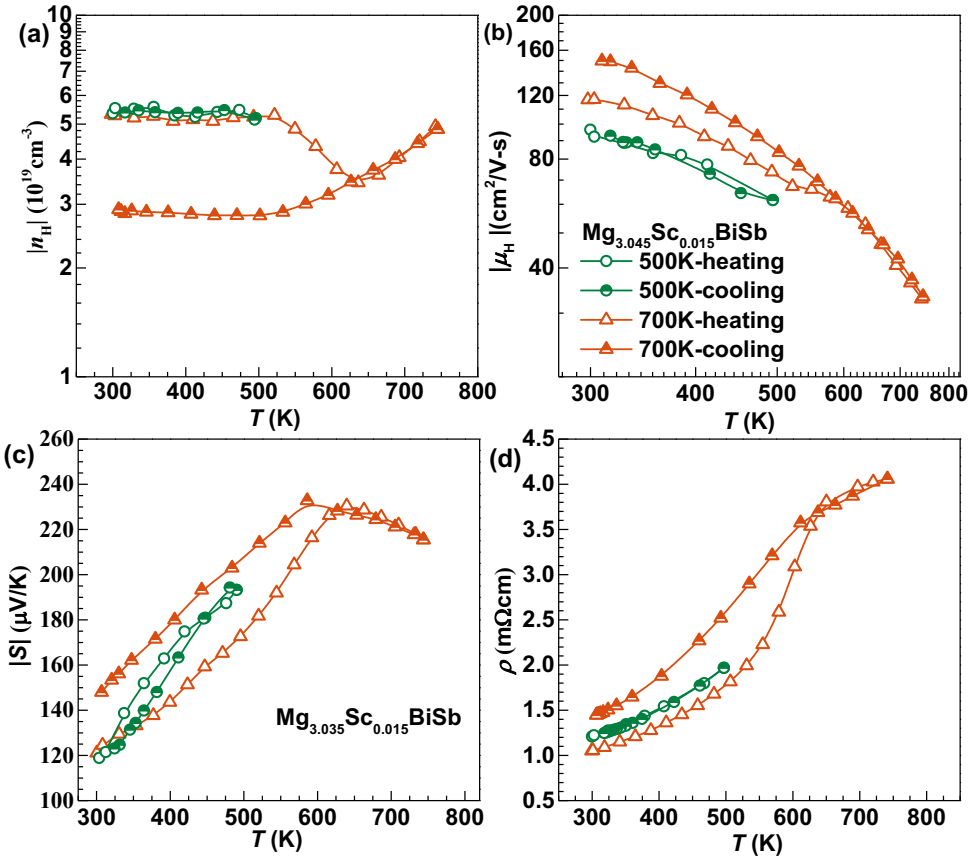

Fig. S2. Temperature dependent (a) Hall carrier concentration (n_H), (b) Hall mobility (μ_H), (c) Seebeck coefficient and (d) resistivity for the high-zT composition $Mg_{3.045}Sc_{0.005}BiSb$ measured up to 500 K and 700 K, respectively.

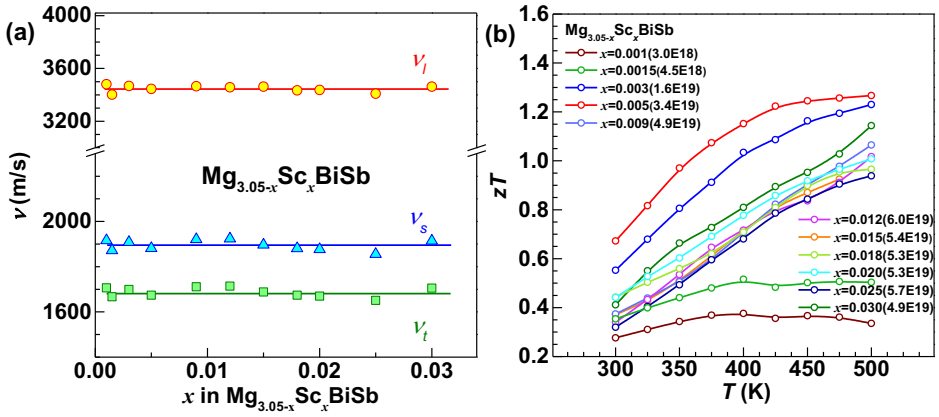

Fig. S3. Room temperature sound velocities (a) and temperature dependent thermoelectric figure of merit, zT (b) for $Mg_{3.05-x}Sc_xSbBi$.

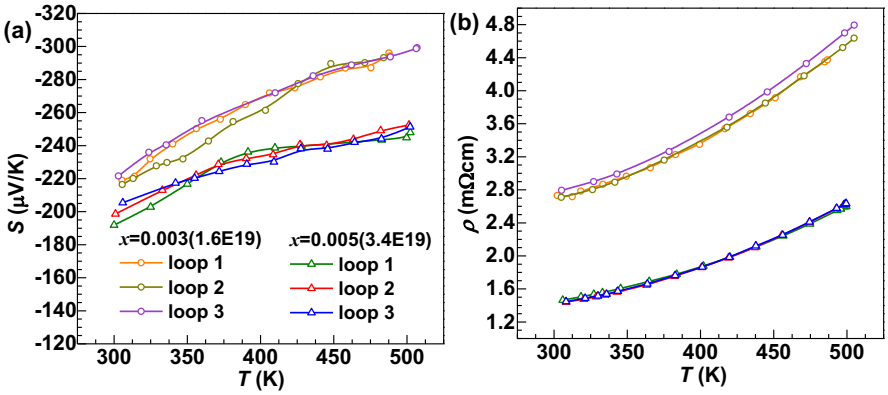

Fig. S4. Temperature dependent Seebeck coefficient (a) and resistivity (b) for $Mg_{3.047}Sc_{0.003}SbBi$ and $Mg_{3.045}Sc_{0.005}SbBi$ showing a good property reproducibility.

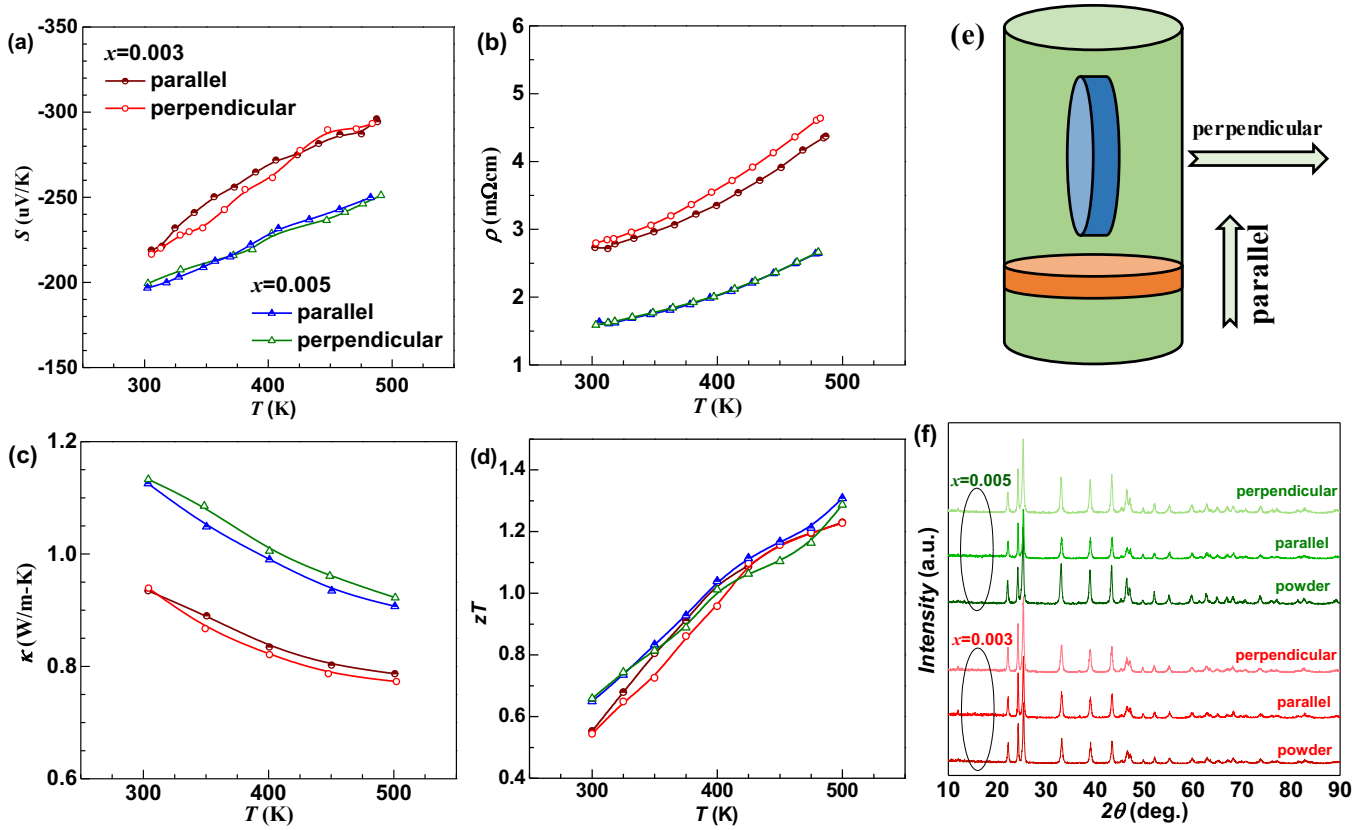

Fig. S5. Temperature dependent Seebeck coefficient (a), resistivity (b), total thermal conductivity (c) and zT (d) along and perpendicular to the hot-press direction (e); and the corresponding XRD patterns room temperature (f).