SUPPLEMENTARY INFORMATION

Unusual consequences of donor and acceptor doping to thermoelectric properties of $MgAg_{0.97}Sb_{0.99}$ alloys

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Table SI. Carrier dopants via substitutions for $MgAg_{0.97}Sb_{0.99}$ alloy, where D is the dopant.

parent	Mg (X_e=1.31, 2+, r=1.36Å)			Ag (X_e=1.93, 1+, r=1.34Å)			Sb (X_e=2.05, 3-, r=1.41 Å)	
dopant	Al	Y	Na[2]	Co	Ni[1]	Cd	Pb	Self (Sb)
X_e	1.61	1.22	0.93	1.88	1.92	1.69	2.33	2.05
valence states	3+	3+	1+	3+, 2+	2+, 3+	2+, 1+	2+	3-
r (Å)	1.18	1.62	1.54	1.16	1.15	1.48	1.47	1.41
carrier type[3]	*n*	*n*	*p*	*n*	*N*	*p*	*n*	*p*
sample	$(Mg_{1-x}D_x)Ag_{0.97}Sb_{0.99}$			$Mg(Ag_{0.97-x}D_x)Sb_{0.99}$			$MgAg_{0.97}(Sb_{0.99-x}D_x)$	$MgAg_{0.97}Sb_{0.99+x}$
substituting level x(at %)	0.50 1.00 5.00	0.25 0.50 1.00 2.50	0.50 0.75 1.00	0.50	0.50	0.50 1.00	0.25 0.50 1.00	0.25 0.50

[1] H. Z. Zhao, J. E. Sui, Z. J. Tang, Y. C. Lan, Q. G. Jie, D. Kraemer, K. N. McEnaney, A. Guloy, G. Chen, and Z. F. Ren, Nano Energy, 2014, **7**, 97.

[2] J. Shuai, H. S. Kim, Y. C. Lan, S. Chen, Y. Liu, H. Z. Zhao, J. H. Sui, and Z. F. Ren, Nano Energy, 2015, **11**, 640.

[3] The carrier type is determined primarily by electronegativity and then valence state as minor correction.

Table SII. The calculated elastic constants c_{11}, c_{12}, c_{13}, c_{44} and c_{66}, bulk modulus B and shear modulus G(all in unit of GPa), Poisson's ratio ν, Debye temperature Θ_D (in unit of K), and Grüneisen parameter γ for MgAgSb compound.

Parameters	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}
Values	115.62	37.88	57.86	96.74	42.04	26.89
Parameters	B	G	ν	Θ_D	γ	
Values	70.58	33.82	0.30	267.44	1.77	