Electronic Supplementary information (ESI)

Influence of In doping on the thermoelectric properties of $AgSbTe_2$ compound with enhanced figure of merit†

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X-ray Fluorescence Spectroscopy Analysis

The chemical composition of the as-prepared ingots was determined using wavelength dispersive X-Ray fluorescence spectroscopy (WD-XRF, Rigaku ZSX primus II).

Table S1.

Nominal Composition	Measured Composition
$AgSbTe_2$	$AgSb_{0.9}Te_{2.01}$
$AgSb_{0.97}In_{0.03}Te_2$	$AgSb_{0.96}In_{0.037}Te_{2.01}$
$AgSb_{0.95}In_{0.05}Te_2$	$AgSb_{0.93}In_{0.06}Te_{2.02}$
$AgSb_{0.93}In_{0.07}Te_2$	$AgSb_{0.91}In_{0.08}Te_{2.02}$

2013- 6-19 17:53

SQX Calculation Result

Sample : AgSbTe2 ..
Application : InAST
Model : Bulk
Date analyzed : 2013- 6-19 17:48
Balance :
Matching library:
File : AgSbTe2 ..

No.	Component	Result	Unit	Det.limit	El.line	Intensity	w/o normal
1	Ag	22.7	mass%	0.0132	Ag-KA	138.4399	24.9196
2	Sb	22.7	mass%	0.0398	Sb-KA	44.9431	24.8338
3	Te	54.6	mass%	0.0468	Te-KA	73.8944	59.7960

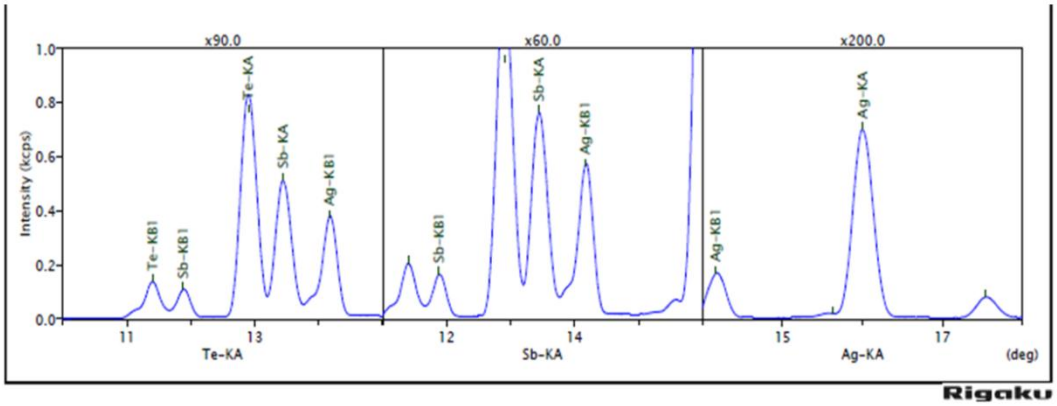


Fig. S1 XRF data for $AgSbTe_2$ sample.

2013-11- 5 22:21

SQX Calculation Result

Sample : In0.03AST
Application : In0.03AST
Model : Bulk
Date analyzed : 2013-11- 5 22:14
Balance :
Matching library:
File : In0.03AST

No.	Component	Result	Unit	Det.limit	El.line	Intensity	w/o normal
1	Ag	22.4	mass%	0.0131	Ag-KA	136.2197	24.4666
2	In	0.418	mass%	0.0205	In-KA	1.5423	0.4569
3	Sb	23.1	mass%	0.0469	Sb-KA	45.8219	25.2652
4	Te	54.1	mass%	0.0524	Te-KA	73.4993	59.0973

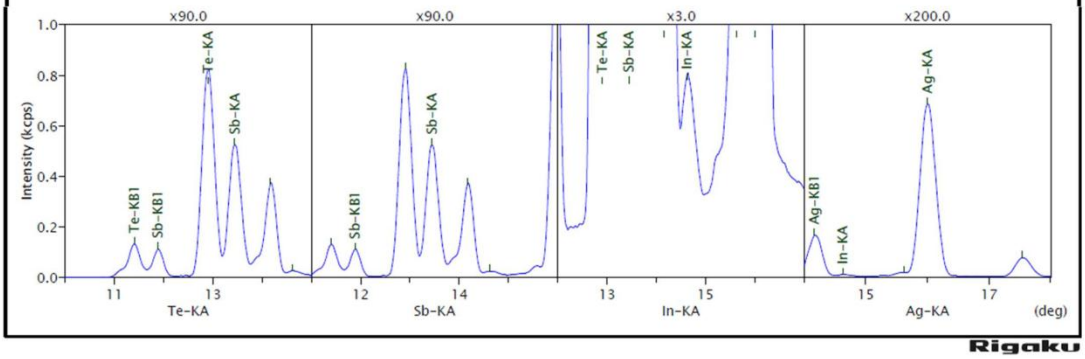


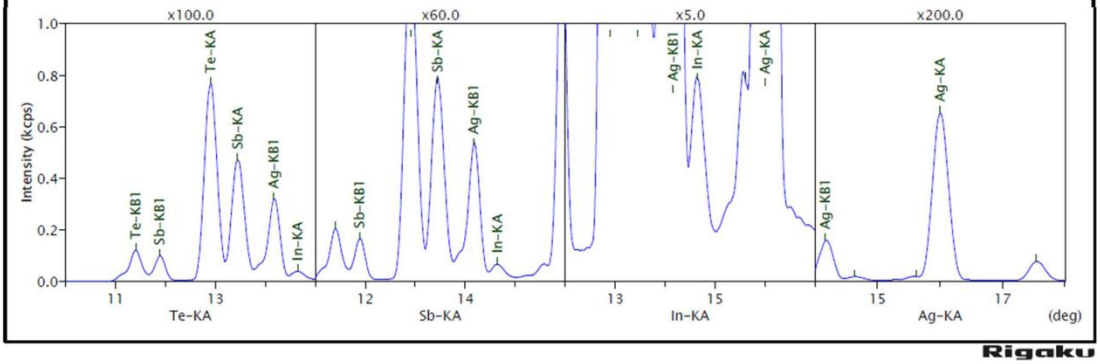
Fig. S2 XRF data for $Ag(Sb_{0.97}In_{0.03})Te_2$ sample.

2013-11- 5 23:17

SQX Calculation Result

Sample : In0.05AST
Application : In0.05AST
Model : Bulk
Date analyzed : 2013-11- 5 23:10
Balance :
Matching library:
File : In0.05AST

No.	Component	Result	Unit	Det.limit	El.line	Intensity	w/o normal
1	Ag	21.1	mass%	0.0134	Ag-KA	129.3453	23.0033
2	In	0.837	mass%	0.0202	In-KA	3.0852	0.9111
3	Sb	22.8	mass%	0.0508	Sb-KA	45.9195	24.8709
4	Te	55.2	mass%	0.0584	Te-KA	75.8323	60.0892



Rigaku

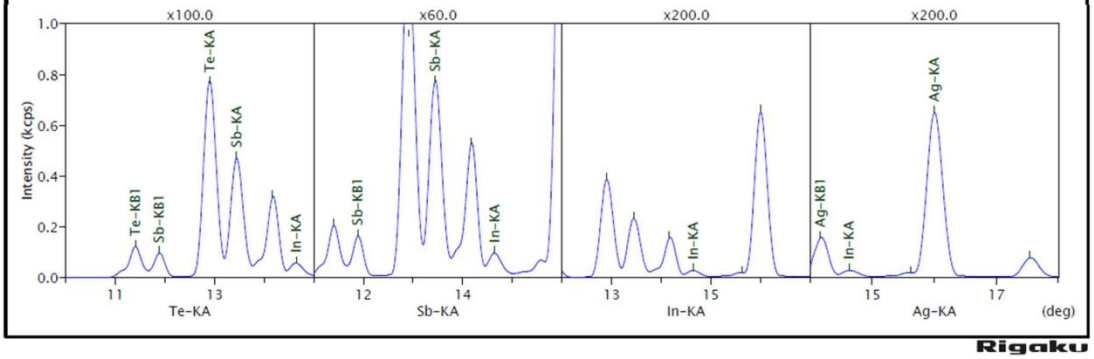
Fig. S3 XRF data for $Ag(Sb_{0.95}In_{0.05})Te_2$ sample.

2013-11- 5 23:00

SQX Calculation Result

Sample : In0.037ST
Application : In0.07AST
Model : Bulk
Date analyzed : 2013-11- 5 22:53
Balance :
Matching library:
File : In0.07AST

No.	Component	Result	Unit	Det.limit	El.line	Intensity	w/o normal
1	Ag	20.9	mass%	0.0130	Ag-KA	128.7740	22.9032
2	In	1.33	mass%	0.0202	In-KA	4.9145	1.4536
3	Sb	22.6	mass%	0.0389	Sb-KA	45.8109	24.7644
4	Te	55.1	mass%	0.0649	Te-KA	76.3907	60.2205



Rigaku

Fig. S4 XRF data for $Ag(Sb_{0.95}In_{0.05})Te_2$ sample.

Seebeck coefficient (α) vs carrier concentration (n_H)

Assuming a single band dominated by acoustic phonon scattering, we express the Seebeck coefficient and electrical conductivity as [1-3]

$$\alpha = \frac{k_B}{e}\left[\frac{2F_1(\zeta F)}{F_0(\zeta_F)} - \zeta_F\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

$$p = \frac{4\pi(2k_BTm^*)^{\frac{3}{2}}}{h^3} F_{\frac{1}{2}}(\zeta_F) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

$$F_j(x) = \int_0^\infty \frac{\zeta_F^j d\zeta_F}{1+\exp(\zeta_F - x)} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

where *Fj(x)* is the Fermi integral, p is the hole concentration, ξ_F is the reduced fermi level, m* is the effective mass, h is the Planck constant and k_B is the Boltzmann constant, respectively.

Calculation of Lorentz number (L)

The Lorenz number L is calculated by the formula as follows [4,5]

$$L = \left(\frac{k_B}{e}\right)^2 \left(\frac{3F_0(\xi)F_2(\xi) - 4F_1^2(\xi)}{F_0(\xi)}\right) \quad (4)$$

where the reduced Fermi energy ξ is obtained from the Seebeck value according to Equation 1. By inserting ξ into Equation 4, L values were calculated to be in the range from 1.71 x10^{-8} to 1.74 x10^{-8} V^2K^{-2}.

References

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5. J. P. Heremans, V. Jovovic, E. S. Toberer, A. Saramat, K. Kurosaki,A. Charoenphakdee, S. Yamanaka and G. J. Snyder, *Science*., 2008, **321**, 554.

Thermal stability

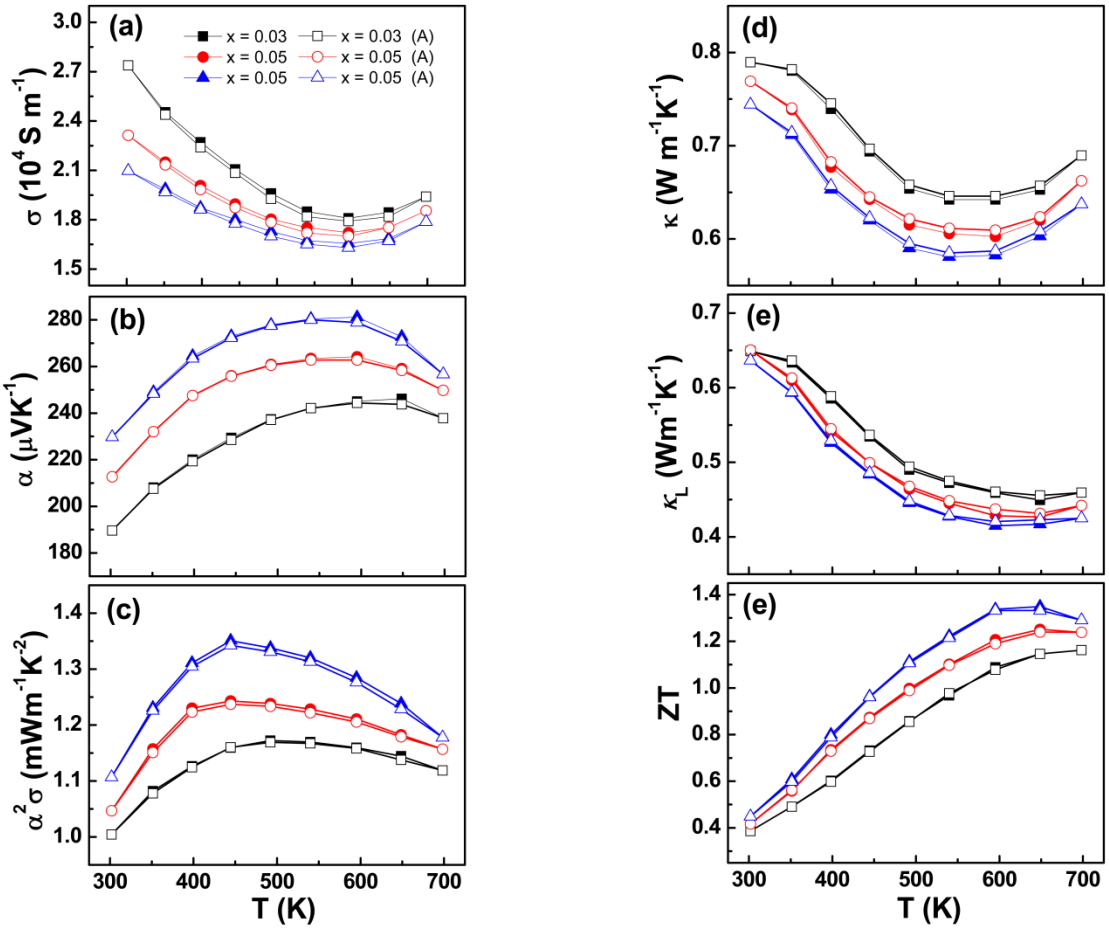

Fig. S5. Temperature dependences of (a) electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) total thermal conductivity, (e) lattice thermal conductivity and (f) thermoelectric figure of merit ZT for samples of $Ag(Sb_{1-x}In_x)Te_2$ (x = 0.03, 0.05, and 0.07). "A" presents the samples annealed at 723 K for 5 days.