

Supplementary Information

Preferential phonon scattering and low energy carrier filtering by interfaces of *in-situ* formed InSb nanoprecipitates and GaSb nanoinclusions for enhanced thermoelectric performance in $\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$

Sanyukta Ghosh¹, Gyan Shankar², Anirudha Karati³, Gerda Rogl⁴, Peter Rogl⁴, Ernst Bauer⁵, B.S. Murty⁶, Satyam Suwas², Ramesh Chandra Mallik^{1,*}

¹Thermoelectric Materials and Devices Laboratory, Department of Physics, Indian Institute of Science, Bangalore 560012, India

²Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India

³Department of Chemistry, Indian Institute of Technology, Madras, Chennai-600036, India

⁴Institute of Materials Chemistry, University of Vienna, Währingerstrasse 42, 1090 Wien, Austria

⁵Institute of Solid State Physics, TU-Wien, Wiedner Hauptstrasse 8-10, 1040 Wien, Austria

⁶Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Madras, Chennai-600036, India

*Corresponding author's E-mail: rcmallik@iisc.ac.in

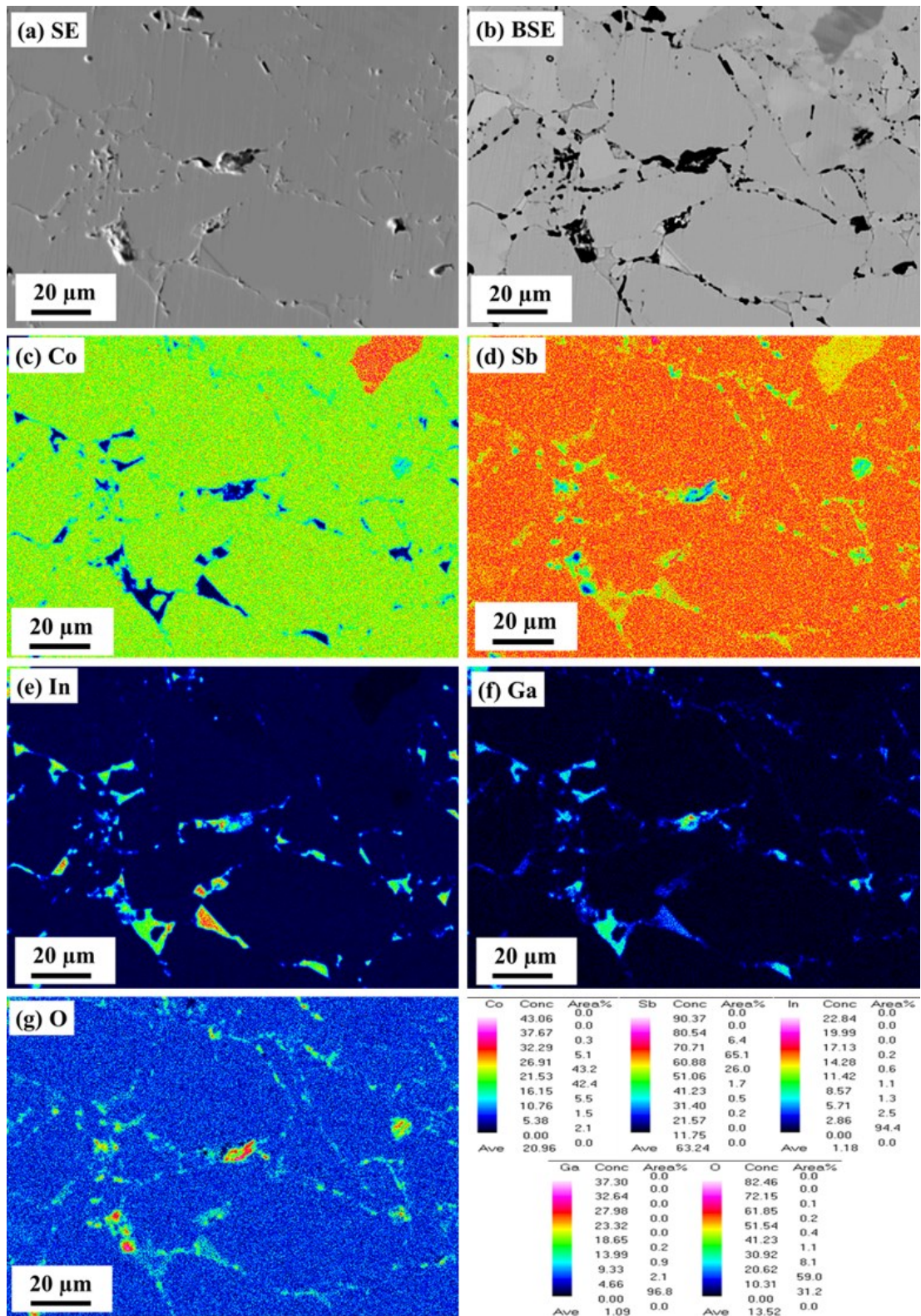


Figure S1 (a)SE micrograph, (b) BSE micrograph of $(\text{GaSb})_{0.2}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$, EPMA-WDS elemental mapping of (c) Co, (d) Sb, (e) In, (f) Ga and (f) O.

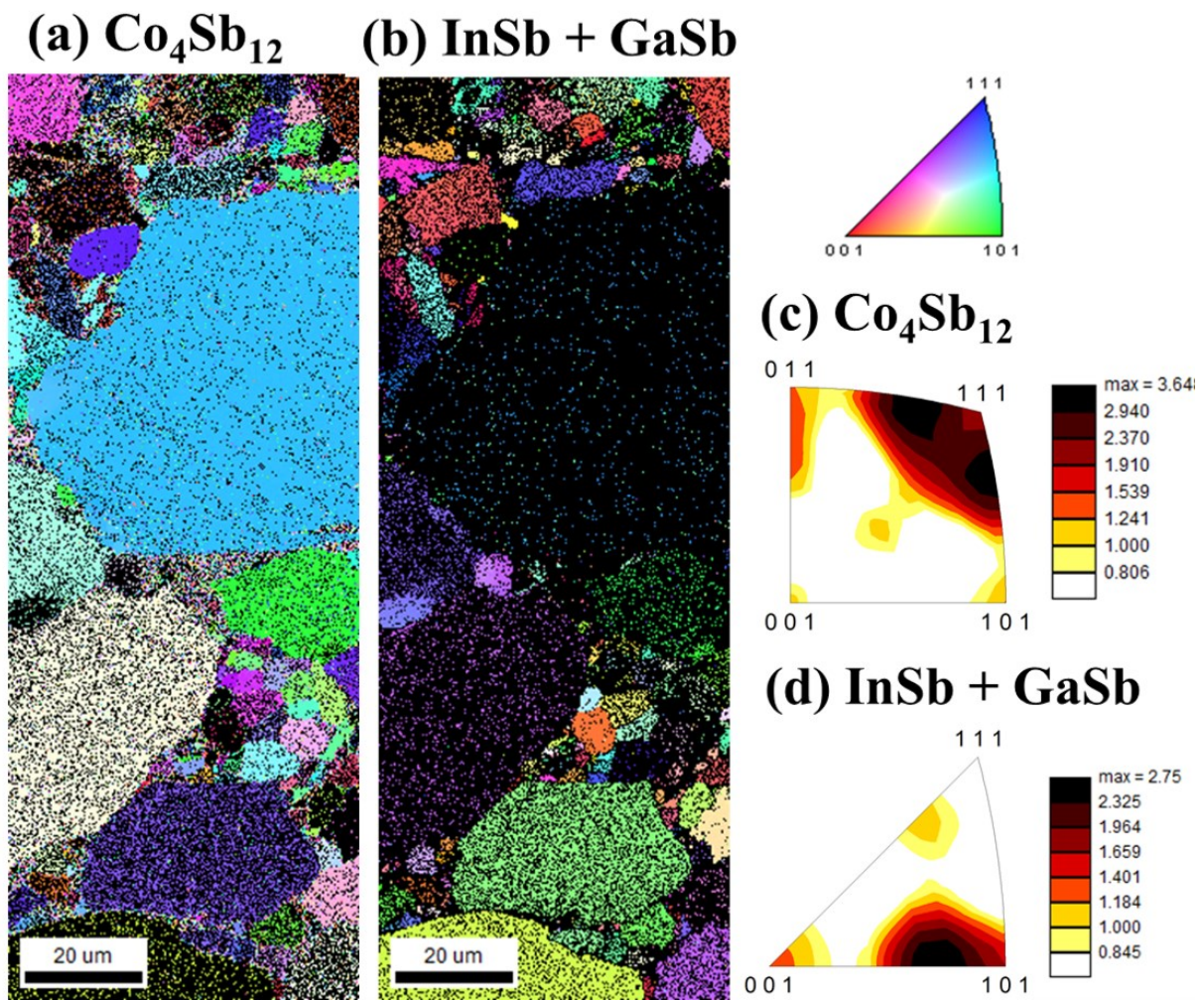


Figure S2 Inverse pole figure (IPF) map of (a) $\text{Co}_4\text{Sb}_{12}$, (b) InSb and GaSb phase showing grain size and their distribution, normal direction (ND) IPF of (c) $\text{Co}_4\text{Sb}_{12}$, (d) GaSb and InSb phase of $(\text{GaSb})_{0.1}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.

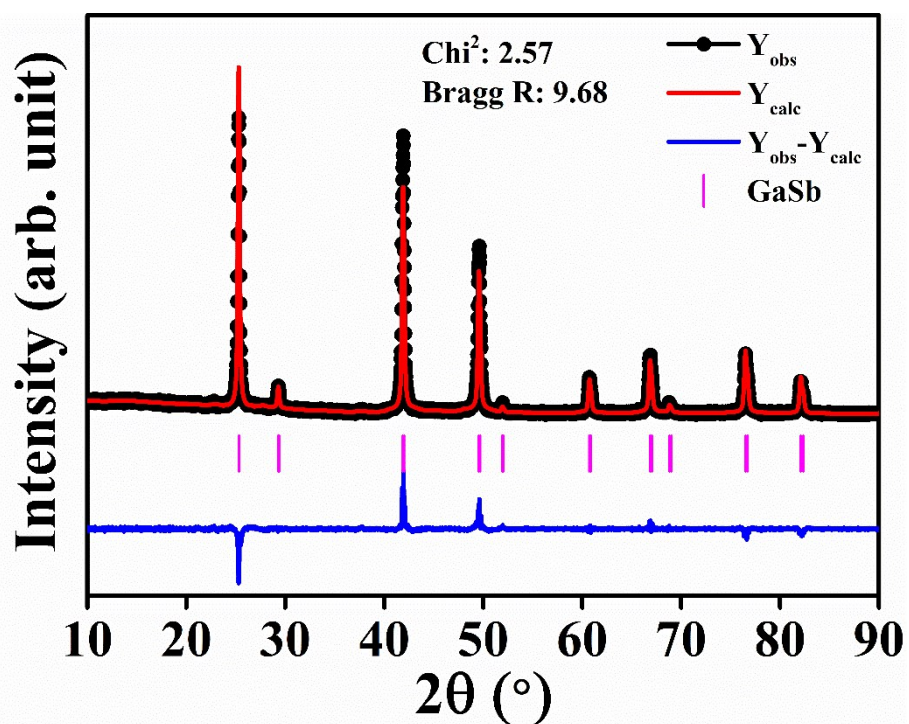


Figure S3 Rietveld refinement analysis of powder XRD pattern of ball-milled GaSb.

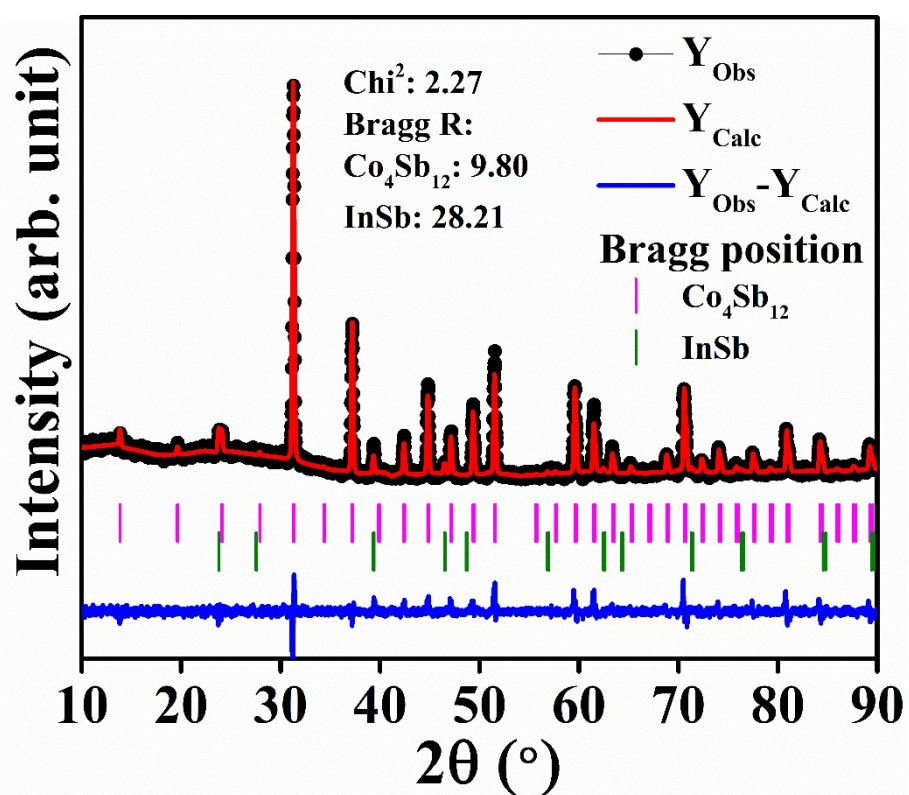


Figure S4 Rietveld refinement analysis of powder XRD pattern of In_{0.2}Co₄Sb₁₂.

Table S1 Rietveld refinement parameters of matrix $\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.

Atom	Wyckoff site	x	y	z	$U_{\text{iso}}(\text{\AA}^2)$	Normalized site occupancy
Co	8c	0.25	0.25	0.25	0.009(1)	1
Sb	24g	0	0.15(7)	0.33(6)	0.005(6)	1
In	2a	0	0	0	0.029(5)	0.24(9)

The composition of the matrix from Rietveld refinement: $\text{In}_{0.24(9)}\text{Co}_4\text{Sb}_{12}$.

Table S2 Rietveld refinement parameters of $(\text{GaSb})_{0.1}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.

Atom	Wyckoff site	x	y	z	$U_{\text{iso}}(\text{\AA}^2)$	Normalized site occupancy
Co	8c	0.25	0.25	0.25	0.004(2)	1
Sb	24g	0	0.15(7)	0.33(5)	0.006(3)	0.97(3)
In	2a	0	0	0	0.068(1)	0.26(4)

The composition of the primary phase of the composite from Rietveld refinement:

$\text{In}_{0.26(4)}\text{Co}_4\text{Sb}_{11.67(9)}$.

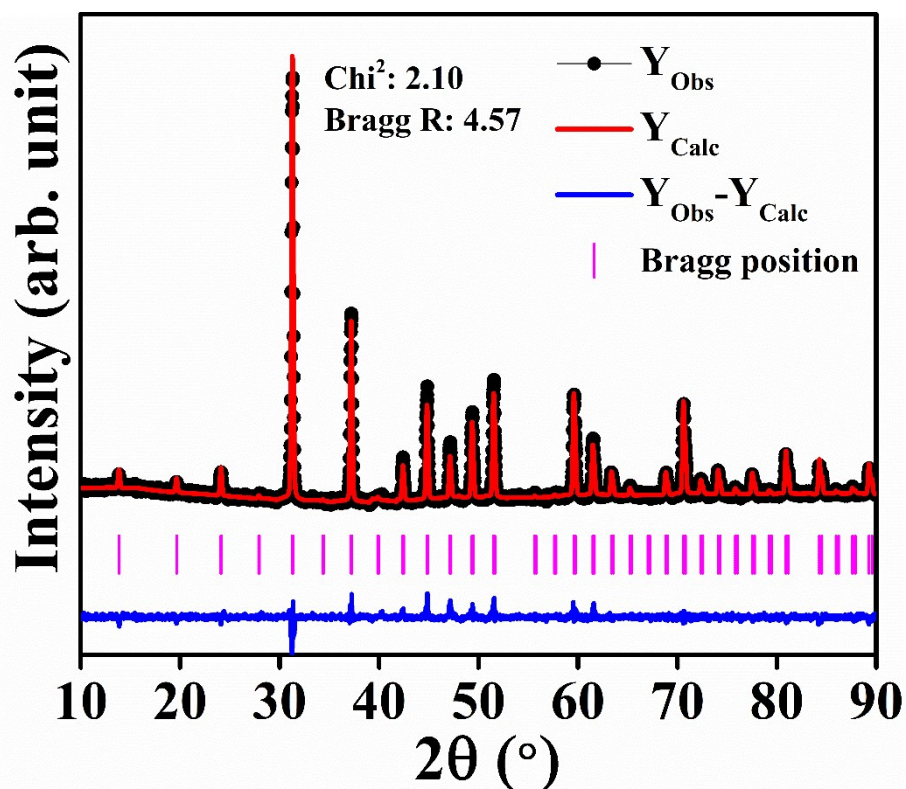
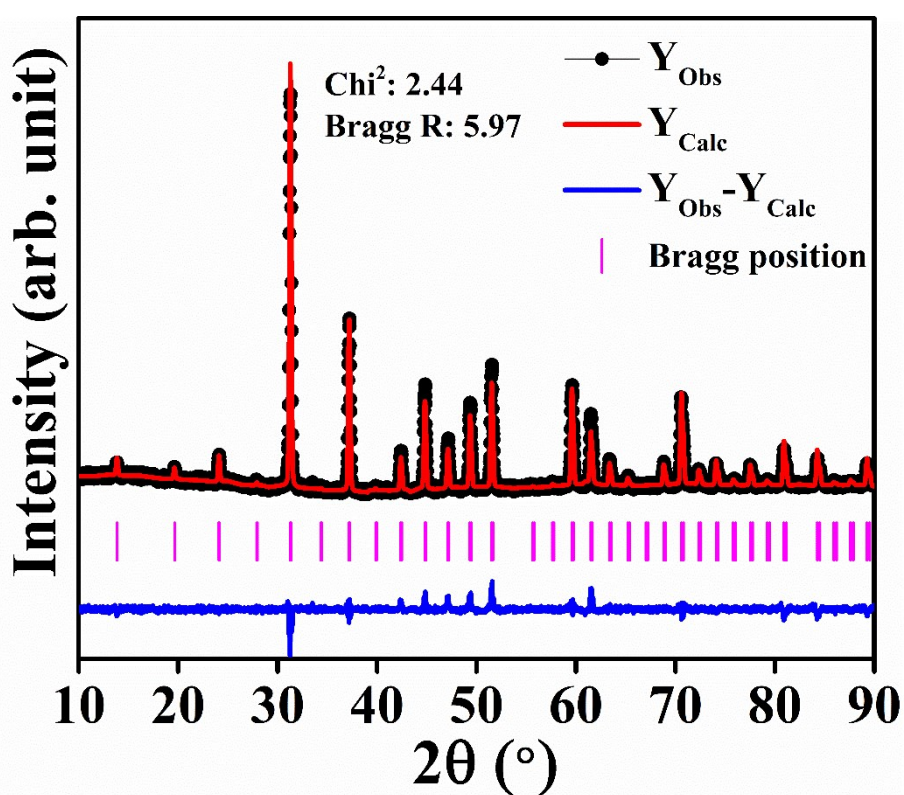
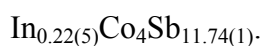
**Figure S5** Rietveld refinement analysis of powder XRD pattern of $(\text{GaSb})_{0.2}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.

Table S3 Rietveld refinement parameters of $(\text{GaSb})_{0.2}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.

Atom	Wyckoff site	x	y	z	$U_{\text{iso}}(\text{\AA}^2)$	Normalized site occupancy
Co	8c	0.25	0.25	0.25	0.006(1)	1
Sb	24g	0	0.15(8)	0.33(4)	0.006(1)	0.97(8)
In	2a	0	0	0	0.043(6)	0.22(5)

The composition of the primary phase of the composite from Rietveld refinement:

**Figure S6** Rietveld refinement analysis of powder XRD pattern of $(\text{GaSb})_{0.3}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.**Table S4** Rietveld refinement parameters of $(\text{GaSb})_{0.3}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.

Atom	Wyckoff site	x	y	z	$U_{\text{iso}}(\text{\AA}^2)$	Normalized site occupancy
Co	8c	0.25	0.25	0.25	0.009(6)	1
Sb	24g	0	0.15(7)	0.33(5)	0.005(3)	0.99(1)
In	2a	0	0	0	0.015(9)	0.23(5)

The composition of the primary phase of the composite from Rietveld refinement:

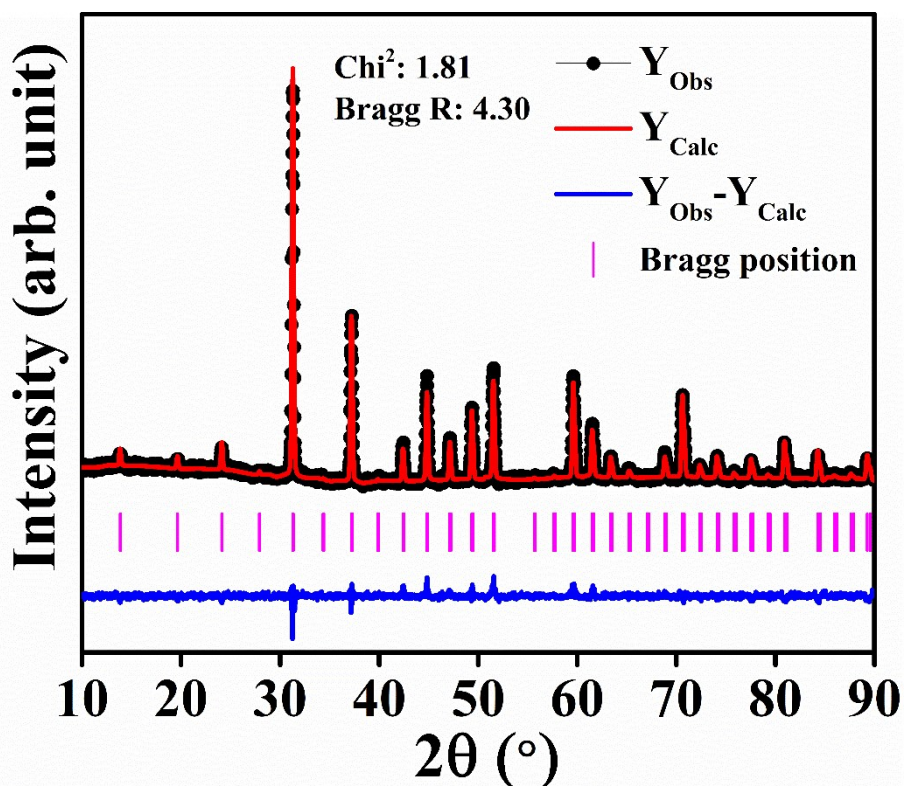
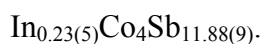
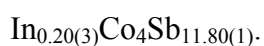


Figure S7 Rietveld refinement analysis of powder XRD pattern of (GaSb)_{0.4}+In_{0.2}Co₄Sb₁₂.

Table S5 Rietveld refinement parameters of (GaSb)_{0.4}+In_{0.2}Co₄Sb₁₂.

Atom	Wyckoff site	x	y	z	U _{iso} (Å ²)	Normalized site occupancy
Co	8c	0.25	0.25	0.25	0.007(5)	1
Sb	24g	0	0.15(7)	0.33(4)	0.006(2)	0.98(3)
In	2a	0	0	0	0.053(9)	0.20(3)

The composition of the primary phase of the composite from Rietveld refinement:



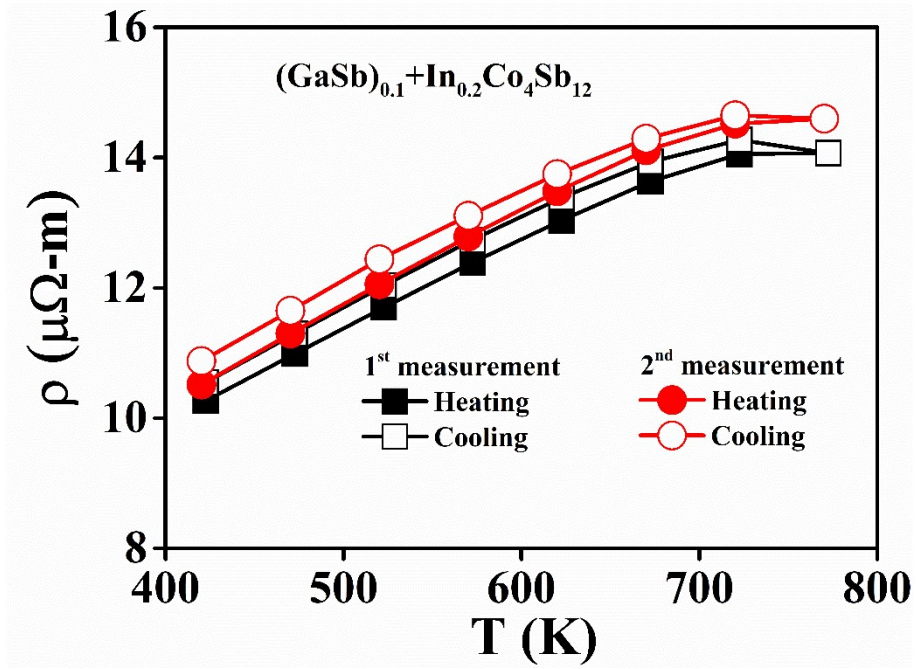


Figure S8 Temperature dependence of electrical resistivity of $(\text{GaSb})_{0.1}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.

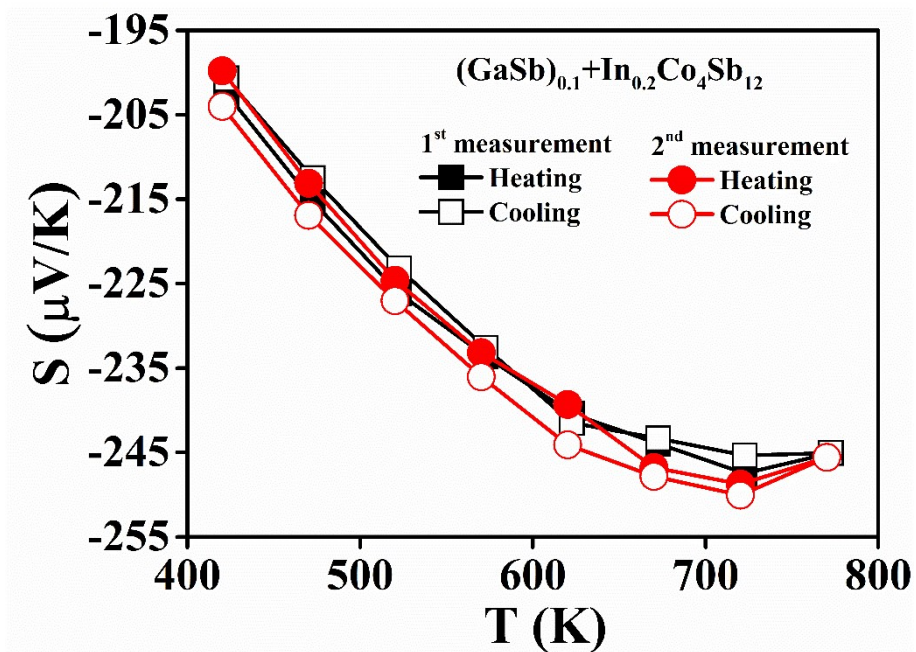


Figure S9 Temperature dependence of Seebeck coefficient of $(\text{GaSb})_{0.1}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.

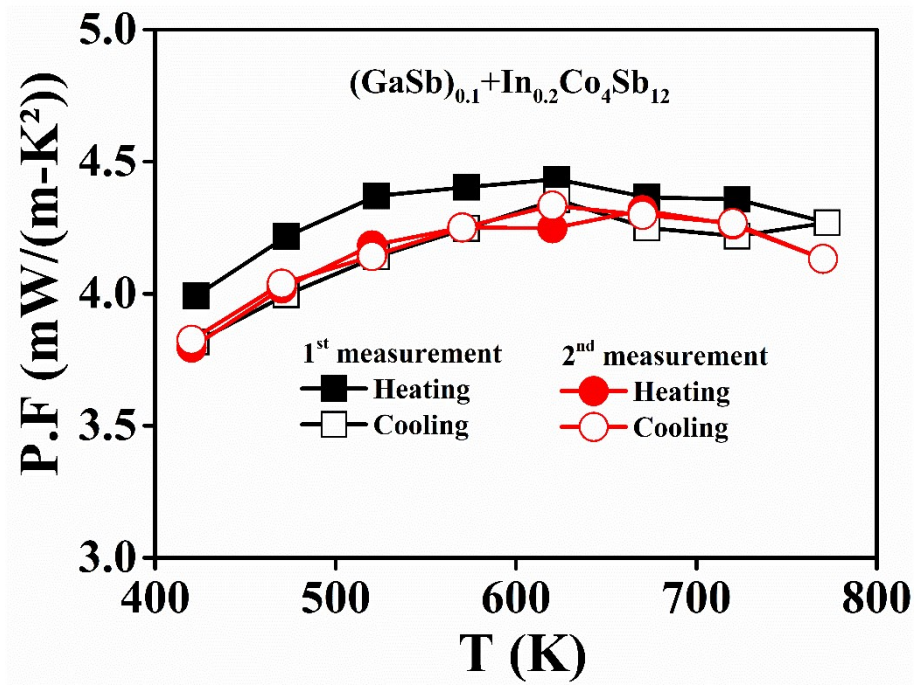


Figure S10 Temperature dependence of power factor of $(\text{GaSb})_{0.1}+\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$.