Supporting Information

Exploring Structure and Thermoelectric Properties of p-type $Ge_{1-x}In_xSb_4Te_7$ Compounds

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Supplementary Text

The theoretical minimum lattice thermal conductivity (κ_{min}) of $GeSb_4Te_7$ was about 0.102 W m^{-1} K^{-1}, which is calculated by using the Cahill's model: [1]

$$\kappa_{min} = \frac{1}{2.48} k_B n^{\frac{2}{3}} (2v_t + v_l)$$

where k_B is the Boltzmann constant (1.38×10^{-23} J/K), n is the number density of atoms (in units of atoms/m^3), v_t and v_l are respectively the transverse and longitudinal sound velocity (m/s).

The atomic number density (n) can be determined by $n = \frac{\rho \cdot N_A}{M}$, where N_A: Avogadro's number (6.022×10^{23} mol^{-1}); ρ: density of the material (kg/m^3); M: molar mass (kg/mol). The calculated density of $GeSb_4Te_7$ is 6150 kg/m^3.

To evaluate the transverse (v_t) and longitudinal (v_l) sound velocity, the elastic moduli (C_{ij}) including six independent elastic constants (GPa) was first calculated for $GeSb_4Te_7$:[2]

$$\begin{bmatrix} 93.710 & 20.754 & 40.894 & -26.995 & 0 & 0 \\ 20.754 & 93.710 & 40.894 & 26.995 & 0 & 0 \\ 40.894 & 40.894 & 82.430 & 0 & 0 & 0 \\ -26.995 & 26.995 & 0 & 58.508 & 0 & 0 \\ 0 & 0 & 0 & 0 & 58.508 & -26.995 \\ 0 & 0 & 0 & 0 & -26.995 & 36.478 \end{bmatrix}$$

Accordingly, longitudinal sound velocity is $v_l = \sqrt{\frac{C_{33}}{\rho}}$ = 3661.04 m/s and transverse sound velocity (polarized perpendicular to the c-axis) is $v_t = \sqrt{\frac{C_{44}}{\rho}}$ = 3084.40 m/s for waves propagating along the c-axis [0001] direction.

References

[1] D. G. Cahill, R. O. Pohl, Lattice vibrations and heat transport in crystals and glasses, Annu. Rev. Phys. Chem. 1988, 39, 93–121.

[2] N. G. Pace and G. A. Saunders, Elastic wave propagation in the group VB semimetals, J. Phys. Chem. Solids 1971, 32, 1585–1601.

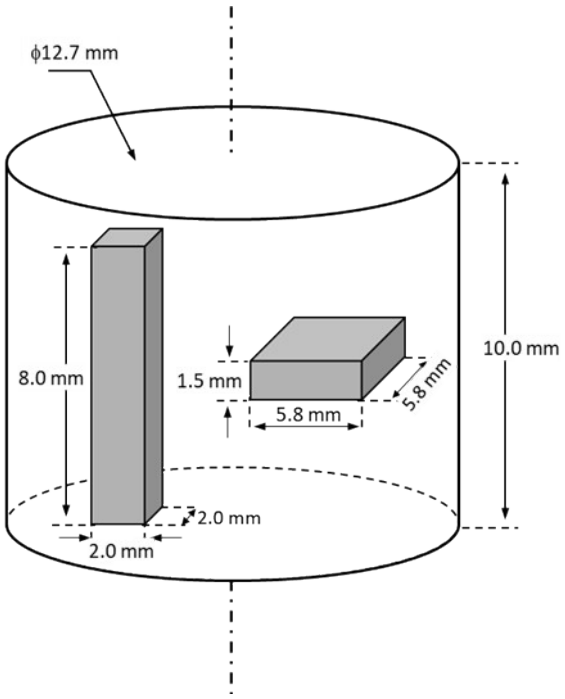

Fig. S1 A schematic drawing illustrates the cuboid specimens obtained from the cylinder-shaped specimens for the measurements of transport properties.

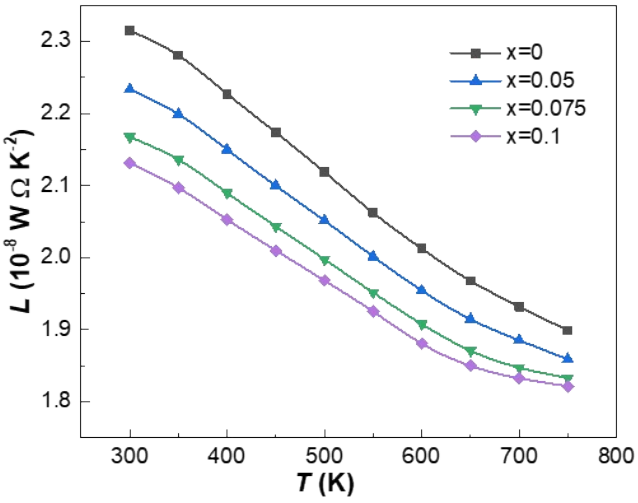

Fig. S2 The Lorentz number (L) estimated from an experimental Seebeck coefficient (S) by $L = 1.5 + \exp\left[-\frac{|S|}{116}\right]$ for $Ge_{1-x}In_xSb_4Te_7$ (x=0, 0.05, 0.075, and 0.1) compounds.

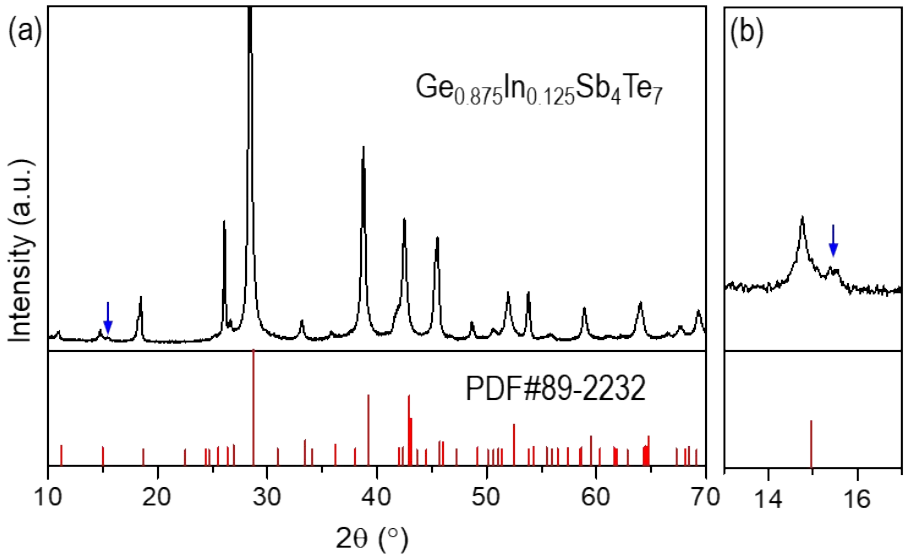

Fig. S3 (a) A typical XRD pattern of powders prepared from $Ge_{0.875}In_{0.125}Sb_4Te_7$ sample. The lattice planes calculated from PDF#89-2232 ($GeSb_4Te_7$) are listed. (b) The zoom-in view shows that apart from (0004) diffraction peak, an extra peak appears as denoted by a vertical arrow, which can be indexed as (0006) diffraction peak of Sb_2Te_3.

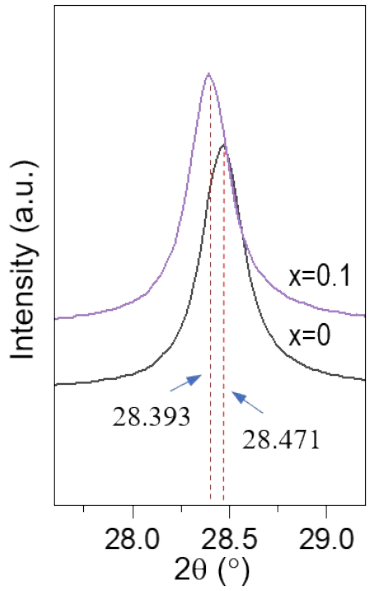

Fig. S4 A zoom-in view of the $(01\bar{1}4)$ diffraction peaks for $GeSb_4Te_7$ and $Ge_{0.9}In_{0.1}Sb_4Te_7$ compounds. The $(01\bar{1}4)$ reflection peaks shift towards lower angles can be discerned. Red vertical broken lines indicate the peak location.