

Supplementary Information

Generation of multi-dimensional defect structures for synergetic engineering of hole and phonon transports: enhanced thermoelectric performance in Sb and Cu co-doped GeTe

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Table S1. Composition, lattice constant, carrier concentration, and DOS effective mass of $\text{Ge}_{1-x-y}\text{Sb}_x\text{Cu}_y\text{Te}$ samples obtained from Hall measurement performed at room temperature.

Nominal composition	Lattice constant		Carrier concentration (10^{20} cm^{-3})	DOS effective mass, m_d^* (m_0)
	a (nm)	c (nm)		
GeTe	0.8316	1.0648	5.69	1.21
$\text{Ge}_{0.9}\text{Cu}_{0.1}\text{Te}$	0.8339	1.0673	6.91	1.18
$\text{Ge}_{0.9}\text{Sb}_{0.1}\text{Te}$	0.8411	1.0491	0.98	1.58
$\text{Ge}_{0.85}\text{Sb}_{0.1}\text{Cu}_{0.05}\text{Te}$	0.8487	1.0331	1.92	1.54
$\text{Ge}_{0.8}\text{Sb}_{0.1}\text{Cu}_{0.1}\text{Te}$	0.8491	1.0324	1.19	1.55

Table S2. Density of $\text{Ge}_{1-x-y}\text{Sb}_x\text{Cu}_y\text{Te}$ samples estimated by applying Archimedes' principle.

Nominal composition	Density (g cm^{-3})
GeTe	6.120
$\text{Ge}_{0.9}\text{Cu}_{0.1}\text{Te}$	6.118
$\text{Ge}_{0.9}\text{Sb}_{0.1}\text{Te}$	6.117
$\text{Ge}_{0.85}\text{Sb}_{0.1}\text{Cu}_{0.05}\text{Te}$	6.117
$\text{Ge}_{0.8}\text{Sb}_{0.1}\text{Cu}_{0.1}\text{Te}$	5.984

S1. Calculation of density-of-states effective mass

We calculated the density-of-states (DOS) effective mass (m_d^*) of $\text{Ge}_{1-x-y}\text{Sb}_x\text{Cu}_y\text{Te}$ samples by using measured Seebeck coefficient (S) and carrier concentration (n) at room temperature based on the following Eq. (S1) [1]:

$$S = \frac{2k_B^2 T}{3eh^2} \left(\frac{\pi}{3n} \right)^{3/2} m_d^* \quad (S1)$$

where k_B , e , and h are the Boltzmann constant, elementary charge, and Planck constant, respectively.

S2. Calculation of Lorentz number L

Under the assumption of the single parabolic band model with acoustic phonon scattering, the Lorentz number (L) can be estimated by using the following Eq. (S2) [2].

$$L = 1.5 + \exp\left(-\frac{|S|}{116}\right) \quad (S2)$$

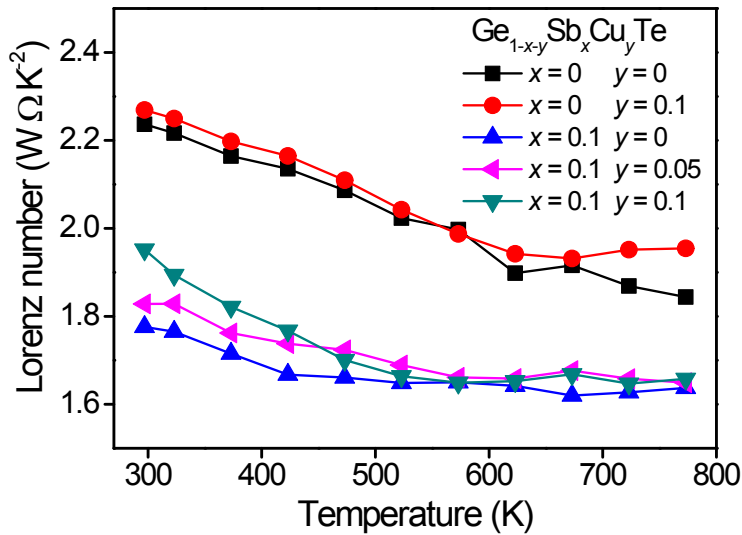


Figure S1. Temperature dependence of the Lorentz numbers of $\text{Ge}_{1-x-y}\text{Sb}_x\text{Cu}_y\text{Te}$ samples.

References

- [1] G.J. Snyder, E.S. Toberer, Nat. Mater. 7 (2008) 105–114.
- [2] H.S. Kim, Z.M. Gibbs, Y. Tang, H. Wang, G.J. Snyder, APL Mater. 3 (2015) 041506.

