Thermoelectric properties of Sn doped p-type Cu_3SbSe_4: a compound with large effective mass and small band gap

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1. XRD patterns

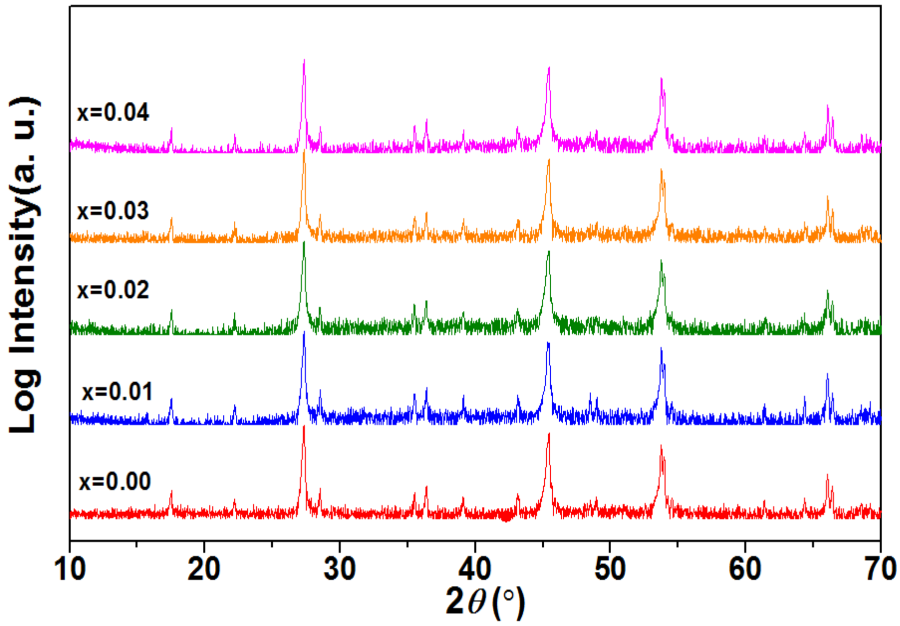

Fig. S1 Enlarged XRD patterns for $Cu_{2.95}Sb_{1-x}Sn_xSe_4$. No peaks corresponding to secondary phases could be seen.

2. Calculation of the Lorenz number by SPB[1,2]

In the SPB model and assuming carriers are mostly scattered by acoustic phonons, the Lorenz number is

$$L=\left(\frac{k_B}{e}\right)^2\frac{3F_0(\eta)F_2(\eta)-4F_1^2(\eta)}{F_0^2(\eta)}, \tag{S1}$$

where $F_n(\eta)=\int_0^\infty \frac{x^n dx}{1+\exp(x-\eta)}$ is the Fermi integrals and η is the reduced chemical potential. Experimentally η is derived from the measured Seebeck coefficient via

$$S = \frac{k_B}{e}\left(\frac{2F_1(\eta)}{F_0(\eta)} - \eta\right) \tag{S2}$$

S and L as functions of η are plotted in Fig. S2 (a).Combining Equations S1 and S2, we can plot the Lorenz number as a function of the measured Seebeck coefficient as demonstrated in Fig. S2 (b).

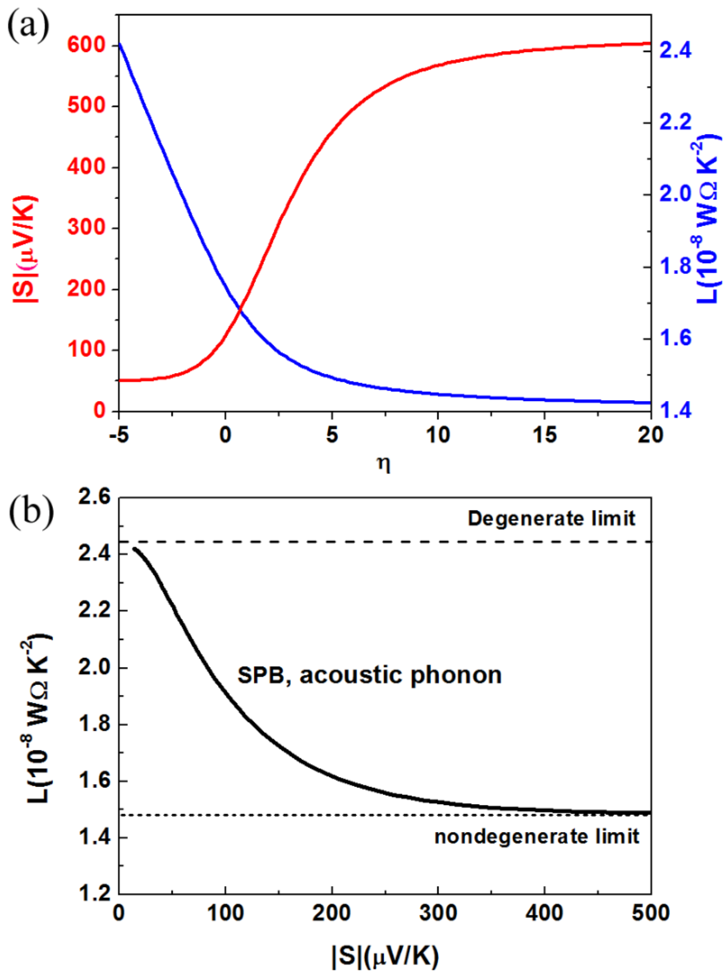

Fig. S2 Calculation results of Lorenz number in the framework of SPB by assuming acoustic phonon scattering limits carriers' mobility: (a) Seebeck coefficient (red) and Lorenz number (blue) as functions of reduced chemical potential and (b) Lorenz number as a function of Seebeck coefficient.

References

[1] G. S. Nolas, J. Sharp and H. J. Goldsmid, *Thermoelectrics: Basic Principles and New Materials Developments*, Springer, Berlin, 2001, pp. 36-42.

[2] Andrew F. May and G. Jeffrey Snyder, in *Materials, Preparation and Characterization in Thermoelectrics*, ed. D. M. Rowe, CRC press, Boca Raton, 2012, chap. 11, pp. 1-18.