Supporting Information

High Thermoelectric Performance of Cu_3SbSe_4 Nanocrystals with $Cu_{2-x}Se$ in-situ Inclusions Synthesized by Microwave-assisted Solvothermal Method

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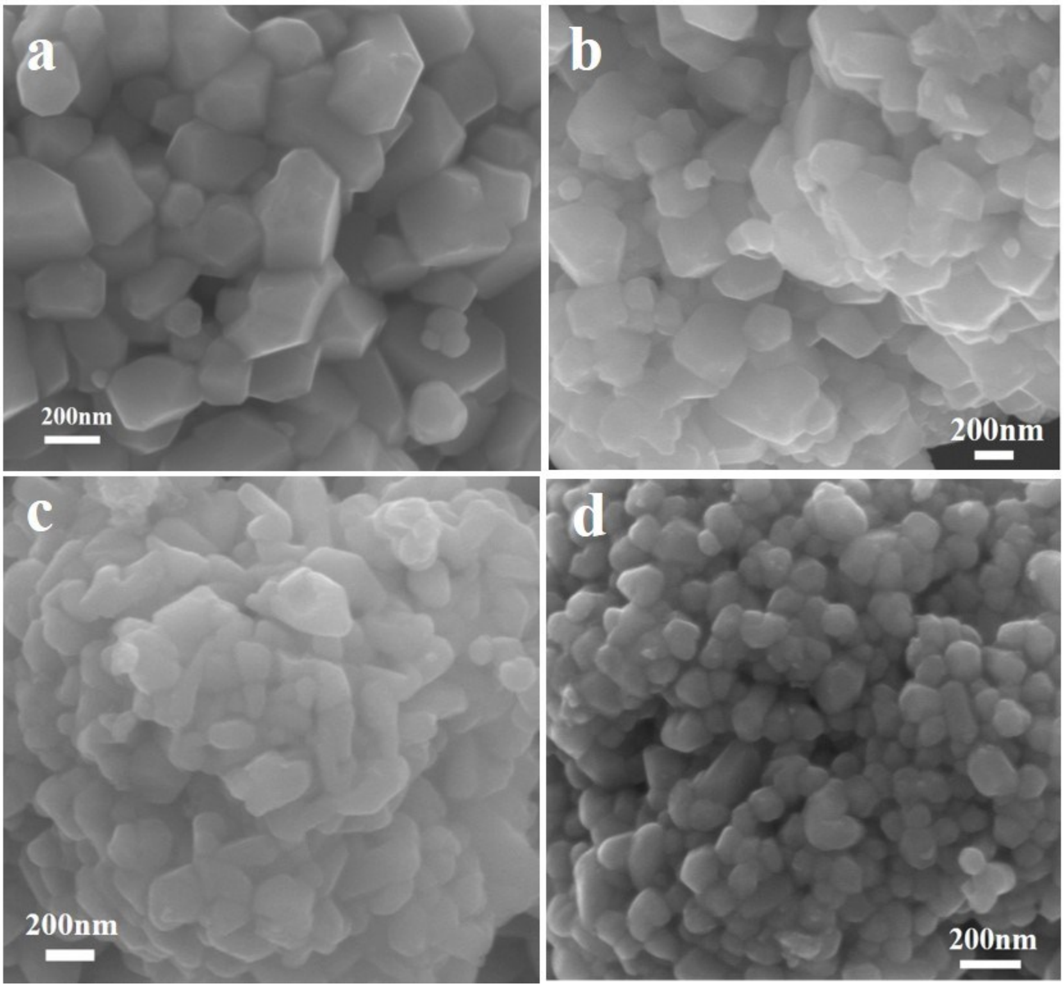


SEM

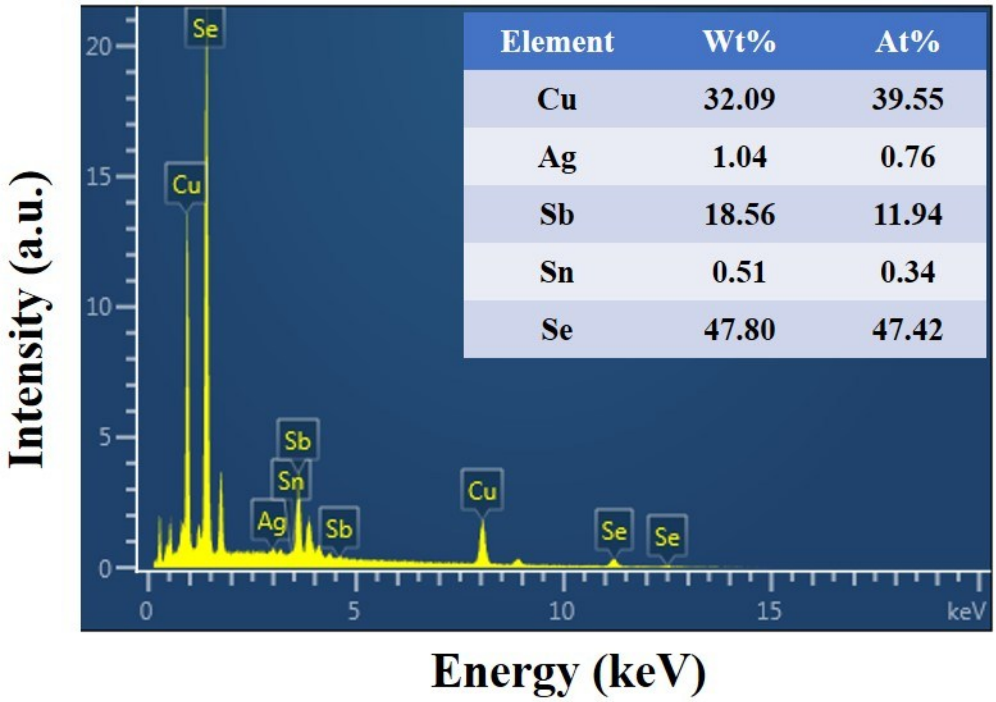
Fig. S1. Representative SEM images of $Cu_{3-y}Ag_ySb_{1-x}Sn_xSe_4$ NCs with (a) $x = 0$, $y = 0$; (b) $x = 0.02$, $y = 0$; (c) $x = 0.03$, $y = 0.1$; (d) $x = 0.05$, $y = 0.2$.

Table S1. Elements distribution of in-situ nanoinclusions.

Element	Wt%	At%	3 Sigma
Ag L	2.47	1.60	0.28
Cu K	59.00	64.50	2.12
Se K	38.53	33.90	10.77
SUM	100	100	

$Cu_{2.8}Ag_{0.2}Sb_{0.95}Sn_{0.05}Se_4$ NCs composition

The nominal composition of $Cu_{2.8}Ag_{0.2}Sb_{0.95}Sn_{0.05}Se_4$ sample is investigated by an energy dispersive spectrometer (EDS) equipped with a JEOL JSM-7800F instrument, and result is given below.



Element	Wt%	At%
Cu	32.09	39.55
Ag	1.04	0.76
Sb	18.56	11.94
Sn	0.51	0.34
Se	47.80	47.42

Fig. S2. Energy dispersive X-ray spectroscopy spectrum for $Cu_{2.8}Ag_{0.2}Sb_{0.97}Sn_{0.03}Se_4$ NCs and the quantitative analysis.

Thermal stability

The electrical properties of a new $Cu_{2.8}Ag_{0.2}Sb_{0.95}Sn_{0.05}Se_4$ sample are measured for two heating-cooling cycles between room temperature and up to 623 K. The results are shown below, which suggest good repeatability. The obtained PF values are even better than that of our previous sample.

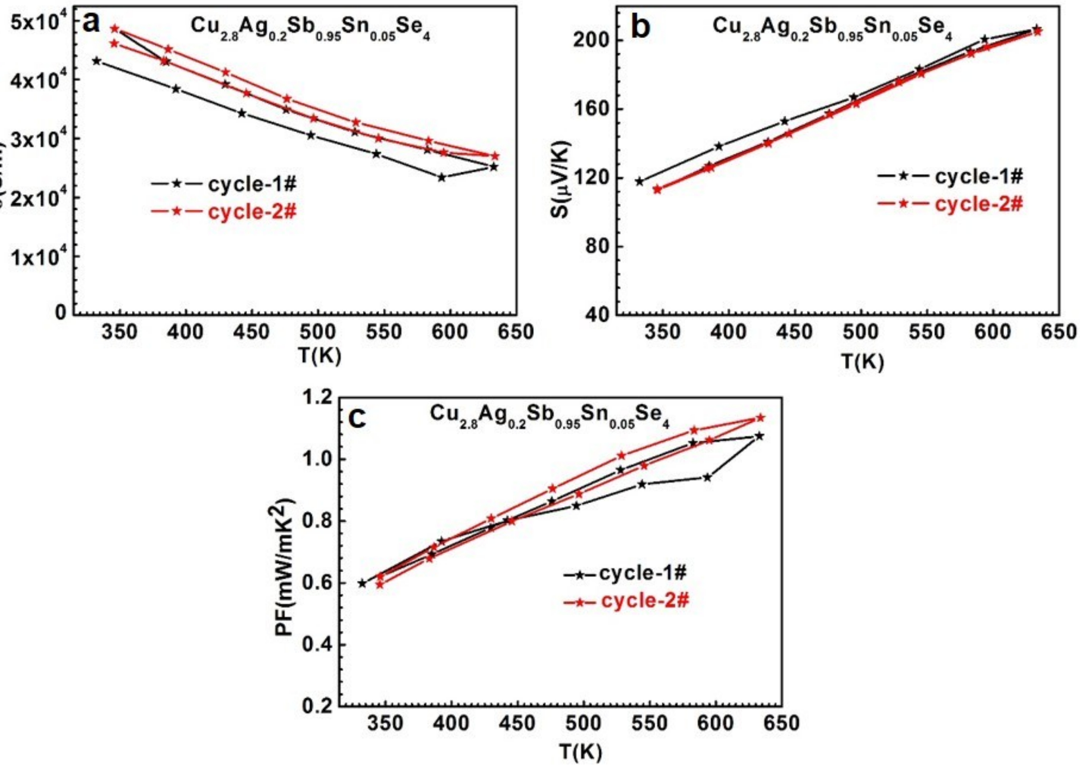


Fig. S3. Electrical properties of the $Cu_{2.8}Ag_{0.2}Sb_{0.95}Sn_{0.05}Se_4$ sample measured for two heating-cooling cycles between room temperature and up to 623 K. (a) electrical conductivity (σ); (b) Seebeck coefficient (S); (c) power factor (PF).

Calculation of the Lorenz number

Lattice thermal conductivity (κ_L) was estimated by subtraction electronic thermal conductivity (κ_e) from total thermal conductivity (κ). κ_e was estimated according to the Wiedemann-Franz law, $\kappa_e = L\sigma T$, where L is the Lorenz number that be estimated by assuming the dominance of acoustic phonon scattering and based on a single parabolic band model within the relaxation time approximation.

The Lorenz number L is calculated from:

$$L = (\frac{k_B}{e})^2\{\frac{\left(r+\frac{7}{2}\right)F_{r+5/2}(\eta)}{\left(r+\frac{3}{2}\right)F_{r+1/2}(\eta)} - [\frac{\left(r+\frac{5}{2}\right)F_{r+3/2}(\eta)}{\left(r+\frac{3}{2}\right)F_{r+1/2}(\eta)}]^2\}$$

$$S = \pm\left(\frac{k_B}{e}\right)[\frac{\left(r+\frac{5}{2}\right)F_{r+3/2}(\eta)}{\left(r+\frac{3}{2}\right)F_{r+1/2}(\eta)} - \eta]$$

$$F_n(\eta) = \int_0^{\infty} \frac{\chi^n}{1+e^{\chi-\eta}} d\chi$$

where η is Fermi energy, k_B is the Boltzmann constant, e is the electron charge and r is the scattering factor, here $r = -1/2$.