

N-type thermoelectric Ag_8SnSe_6 with extremely low lattice thermal conductivity by replacing Ag with Cu

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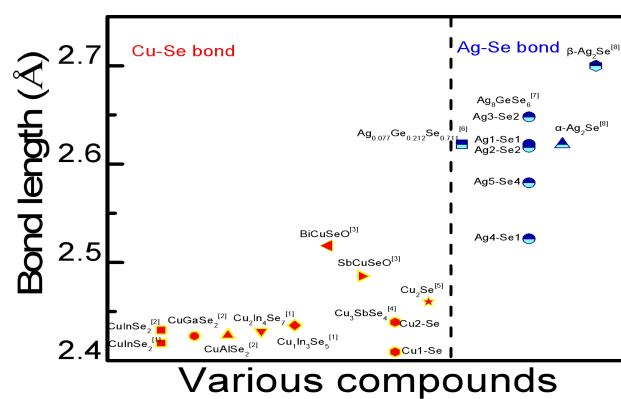


Figure S1. The bond length of Ag-Se and Cu-Se for various compounds.

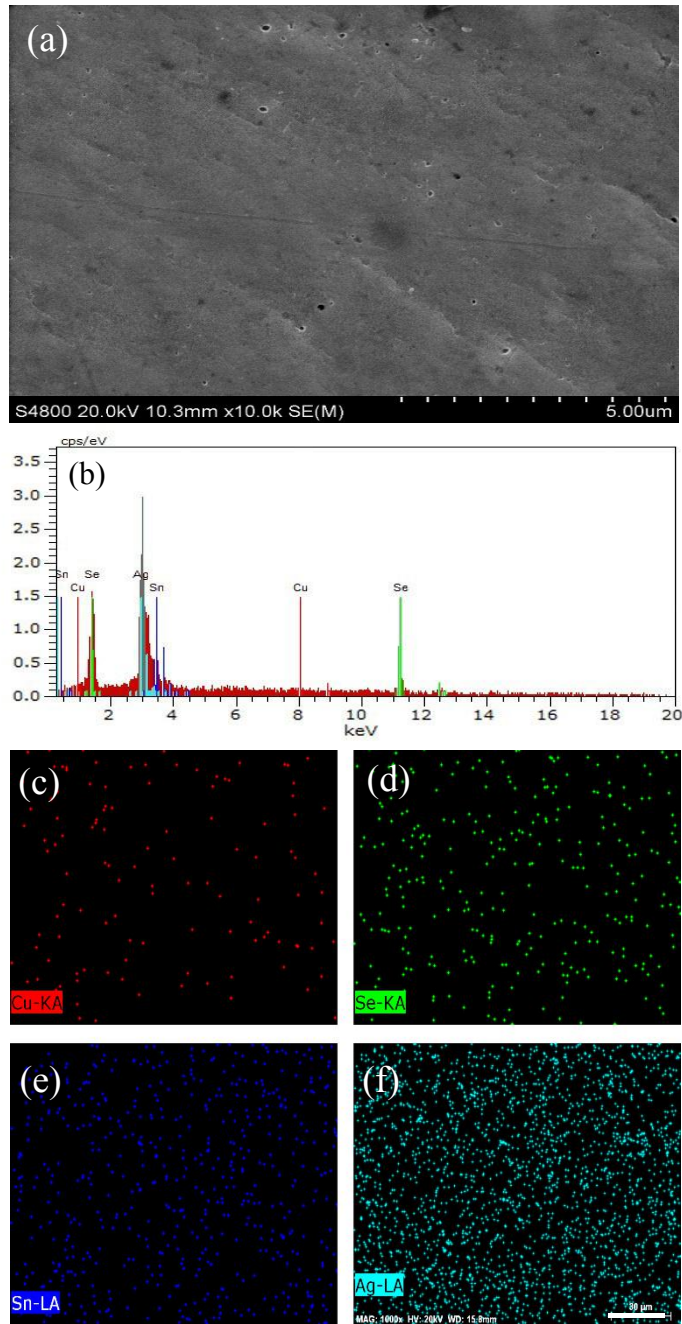


Figure S2. (a) SEM image of the freshly fractured surface of the sample at $x=0.05$; (b) EDS patterns with $x=0.05$ (c-f) EDS mappings of the elements for the bulk sample in $\text{Ag}_{8-x}\text{Cu}_x\text{SnSe}_6$ ($x=0.05$).

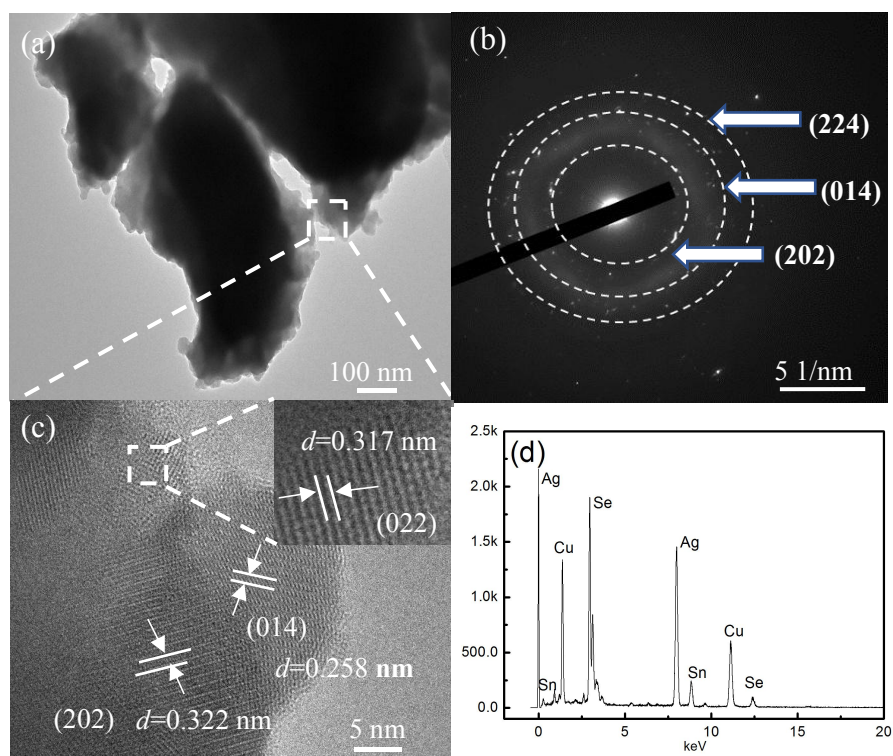


Figure S3. High resolution transmission electron microscopy (HRTEM) image observed in $\text{Ag}_{7.95}\text{Cu}_{0.05}\text{SnSe}_6$. (a) TEM image; (b) Selected area electron diffraction (SAED) pattern; (c) The corresponding high resolution TEM image. An inset is the magnified high resolution TEM image; (d) EDAX result.

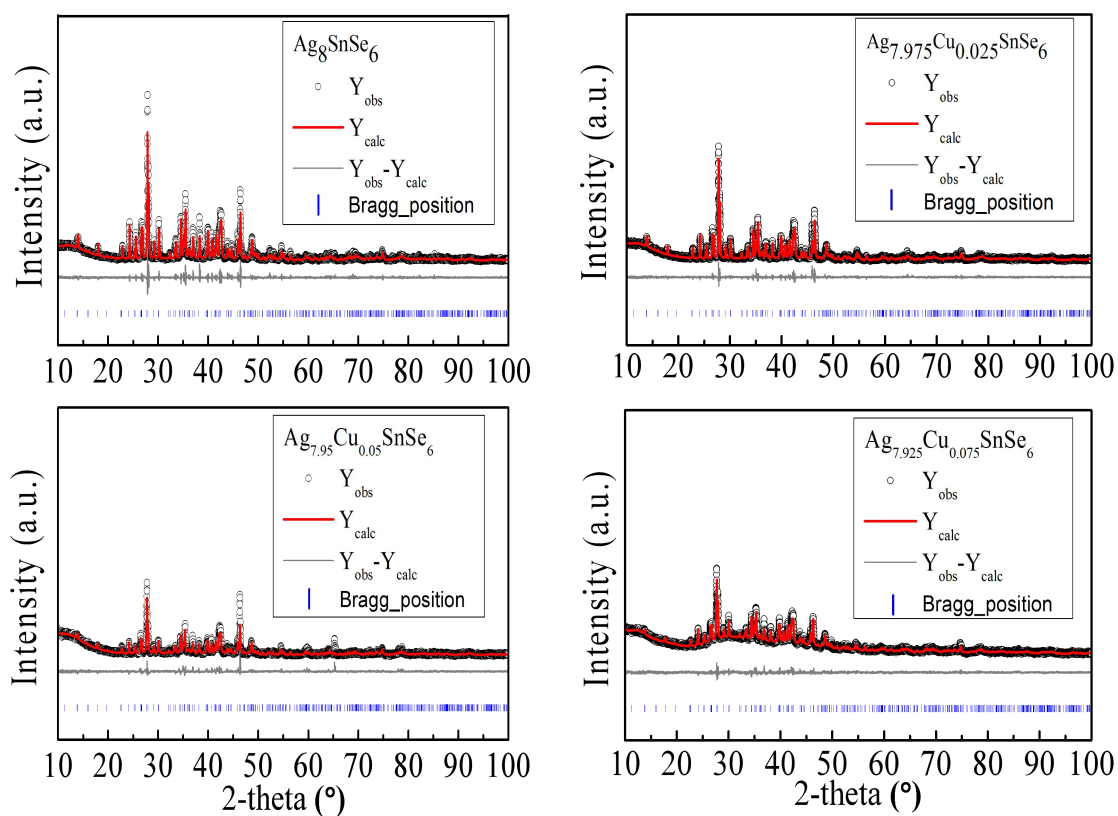


Figure S4. Rietveld refinement using the X-ray diffraction data for the samples $\text{Ag}_{8-x}\text{Cu}_x\text{SnSe}_6$ ($x=0, 0.025, 0.05$ and 0.075).

Table S1. Experimental Parameters of Power X-ray Diffraction, and Refined Crystallographic Data of $\text{Ag}_{8-x}\text{Cu}_x\text{SnSe}_6$ ($x=0, 0.025, 0.05$ and 0.075).

Chemical Formula	Ag_8SnSe_6 ($x = 0$)	$\text{Ag}_{7.975}\text{Cu}_{0.025}\text{SnSe}_6$ ($x = 0.025$)	$\text{Ag}_{7.95}\text{Cu}_{0.05}\text{SnSe}_6$ ($x = 0.05$)	$\text{Ag}_{7.925}\text{Cu}_{0.075}\text{SnSe}_6$ ($x = 0.075$)
a (Å)	7.9180 (6)	7.9160 (6)	7.9151 (10)	7.9164 (5)
b (Å)	7.8243 (6)	7.8226 (6)	7.8247 (10)	7.8225 (5)
c (Å)	11.0505 (8)	11.0463 (8)	11.0462 (14)	11.0448 (6)
V (Å ³)	684.61 (8)	684.03 (8)	648.12 (15)	683.96 (7)
$^a R_B$ (%)	2.565	6.6	2.565	2.565
$^b R_p$ (%)	6.87	6.35	7.11	4.52
$^c R_{wp}$ (%)	9.26	8.80	9.94	5.8
$^d S$	1.09	1.09	1.09	1.09

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