Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Effect of annealing temperature on the phase transition, band gap and thermoelectric properties of Cu_2SnSe_3

Siyar Muhammad[1,2], Jun-Young Cho[1], Yong Youn[1], Seungwu Han[1], Miyoung Kim[1], Sung-Hwan Bae[3], Chan Park*[1, 4]

[1] Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Republic of Korea

[2]School of Chemical and Material Engineering, NUST, H-12, Islamabad, Pakistan

[3]Department of Nano Science and Engineering, Kyungnam University, Changwon, 51767, Republic of Korea

[4] Research Institute of Advanced Materials, Seoul National University, Seoul 08826, Republic of Korea

*Corresponding Author: pchan@snu.ac.kr

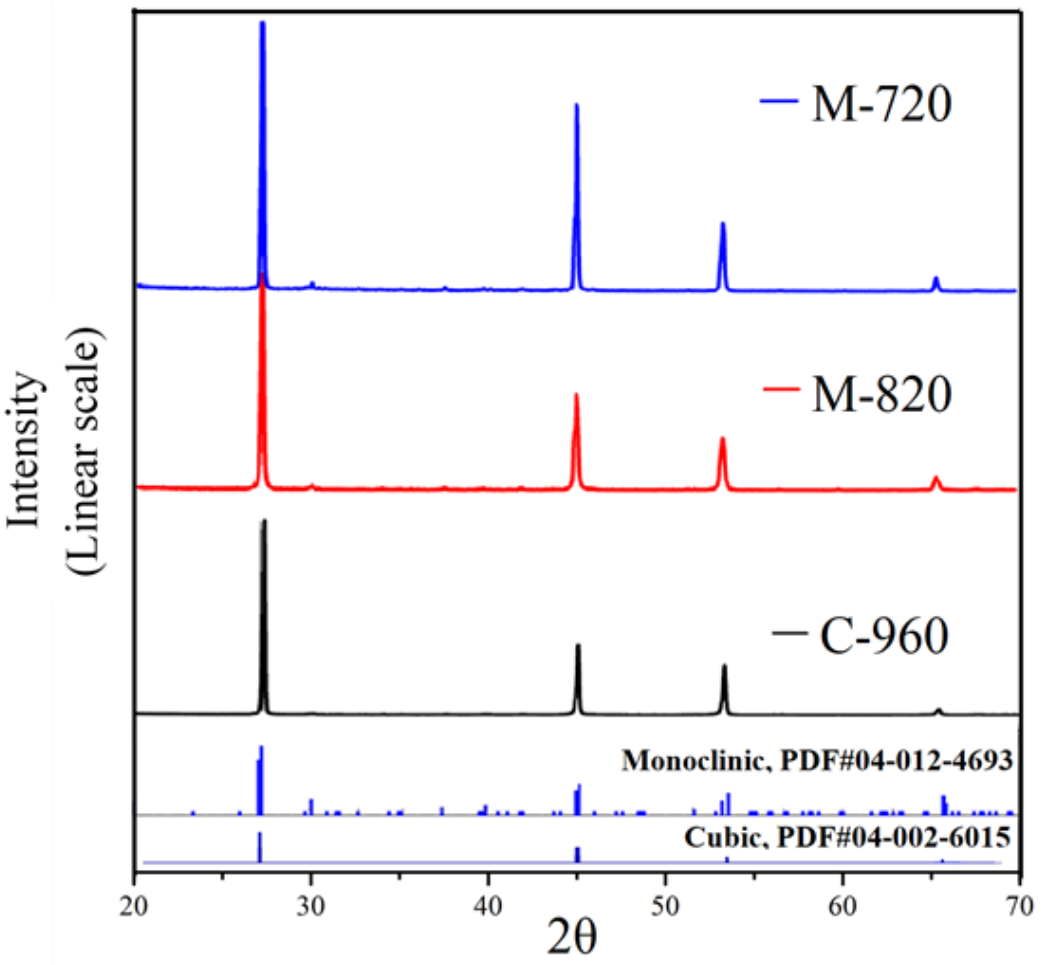


Figure S1. XRD patterns of Cu_2SnSe_3 powder samples annealed at 720 K (M-720), 820 K (M-820) and 960 K (C-960) after melting in evacuated quartz ampoule followed by water quenching. M refers to the mostly monoclinic phase while C refers to the mostly cubic phase Cu_2SnSe_3. The bottom two lines represent the reference spectra (PDF card) of the cubic and monoclinic phases of Cu_2SnSe_3.

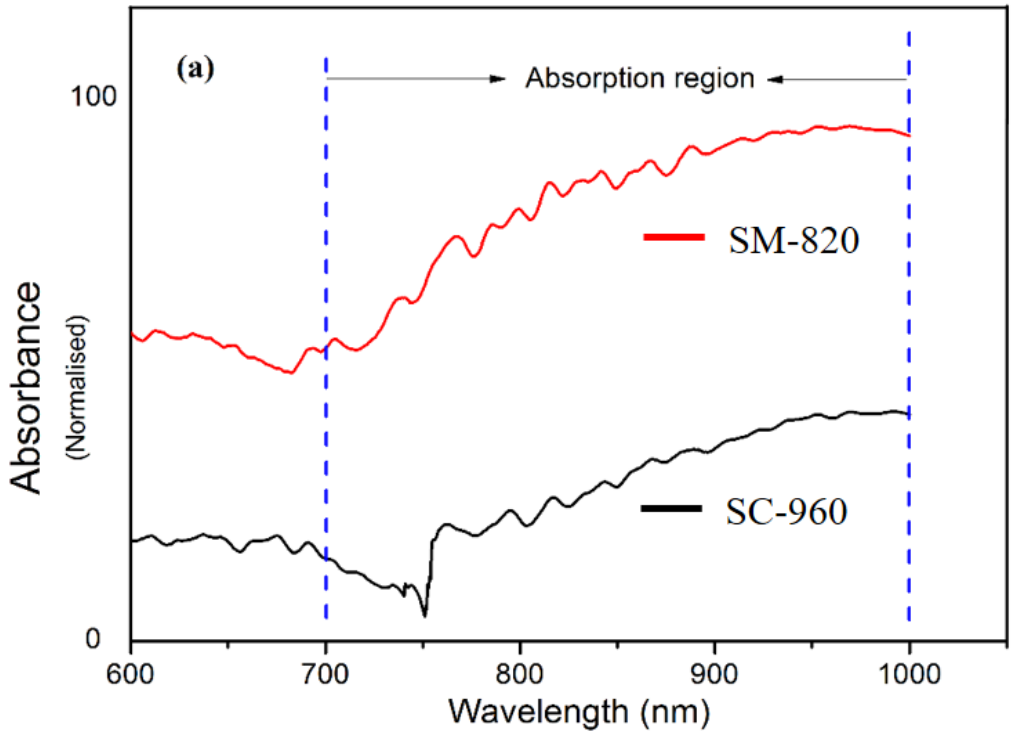


Figure S2. shows the optical absorption spectra obtained from the UV-Vis spectroscopy for the SM-820 and SC-960 samples.

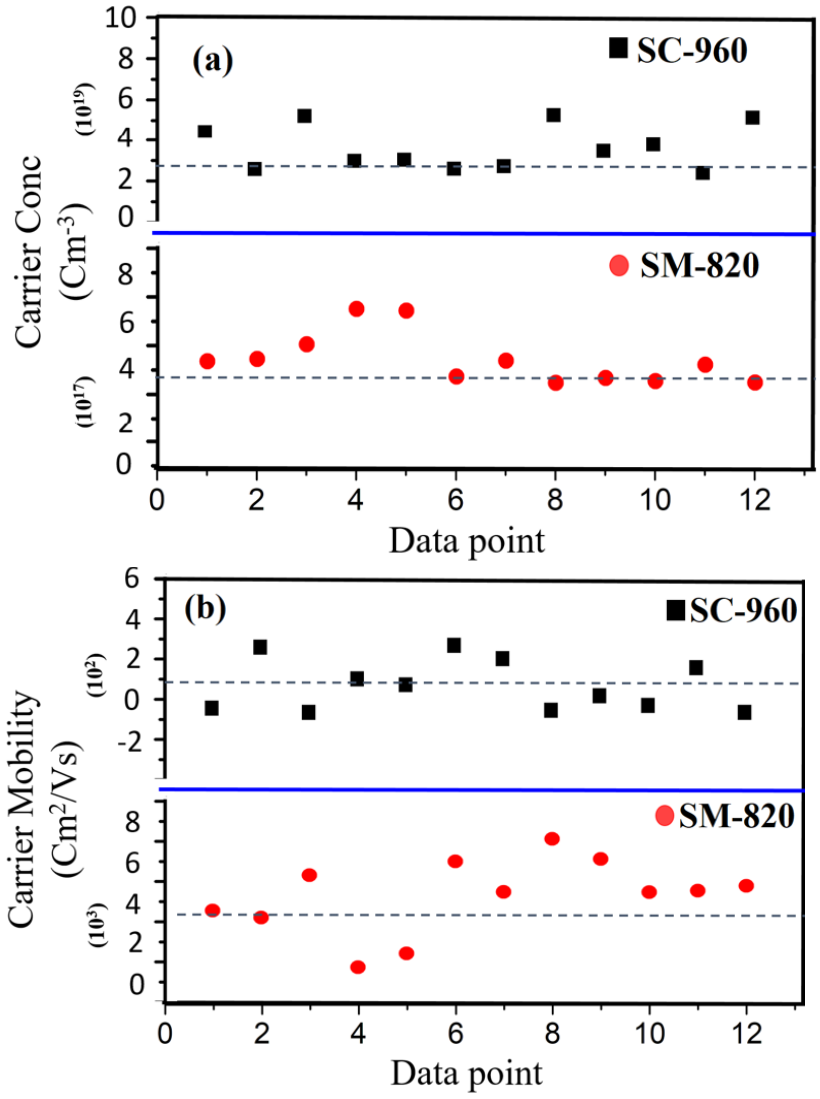
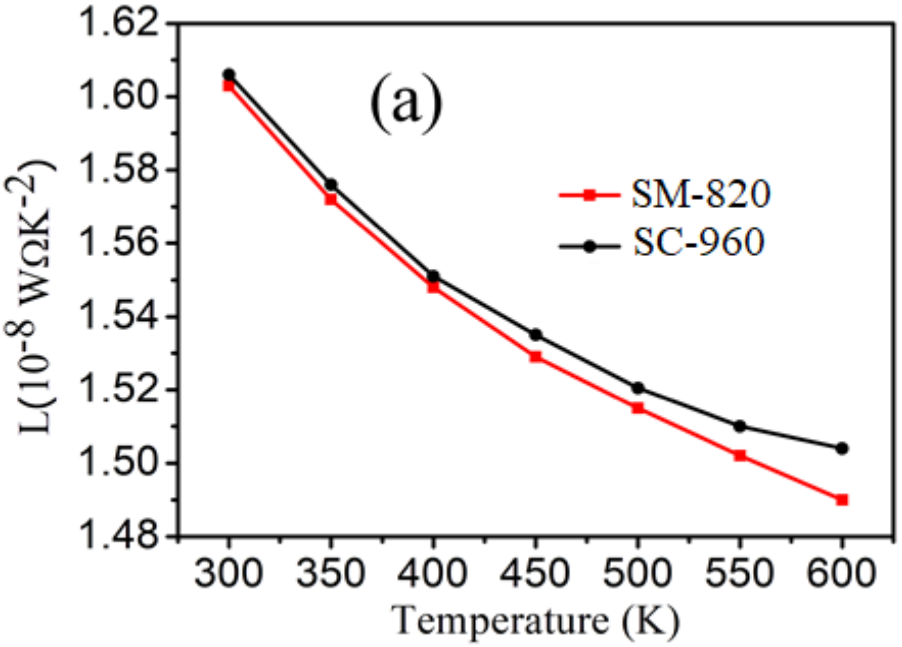
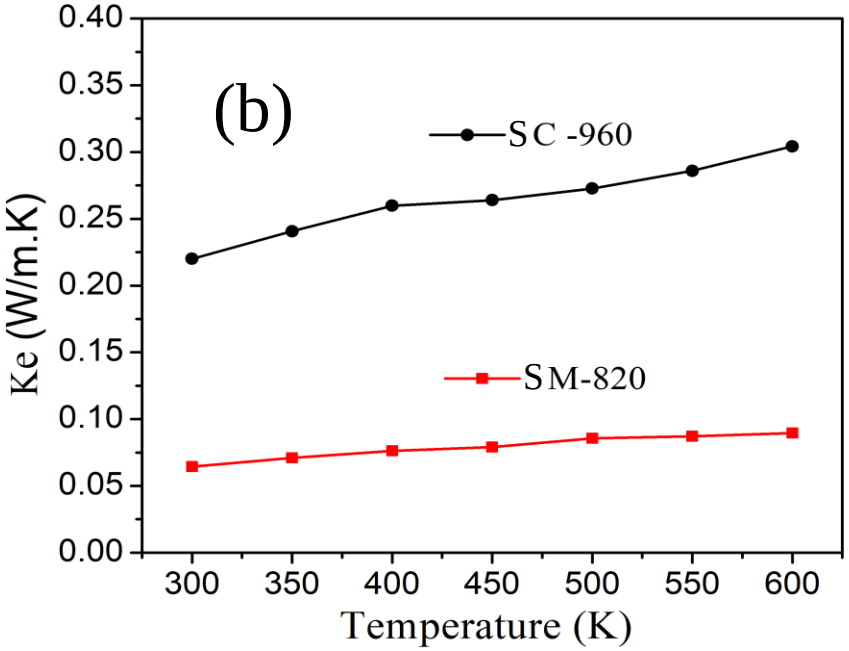


Figure S3. (a) Hole concentration and (b) carrier mobility of SM-820 (square points) and SC-960 (circle points), measured at room temperature. The results of Hall measurement which were taken 12 times from each sample, show slight deviation from the mean value (dash line). One of the reasons for non-consistent data is the high electrical conductivity of Cu_2SnSe_3, where a slight fluctuation in applied voltage can result in deviation of the measured values.


(a)
SM-820
SC-960
L(10-8 WΩK-2)
Temperature (K)
1.62
1.60
1.58
1.56
1.54
1.52
1.50
1.48
300
350
400
450
500
550
600


(b)
SC -960
SM-820
Ke (W/m.K)
Temperature (K)
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
300
350
400
450
500
550
600

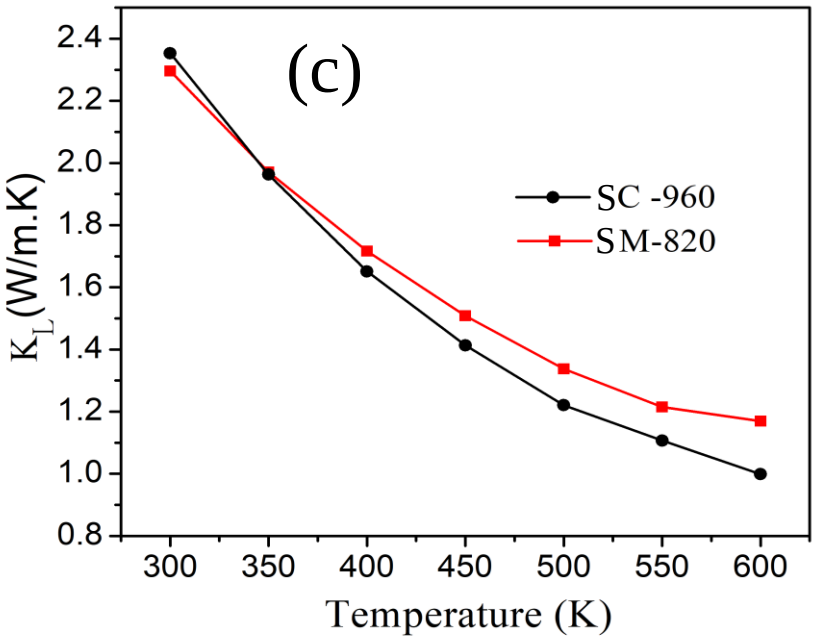


Figure S4. Temperature dependence of (a) Lorenz numbers used for the calculation, (b) thermal conductivity due to carrier transport and (c) lattice part of the thermal conductivity for the SM-820 and SC-960 samples.

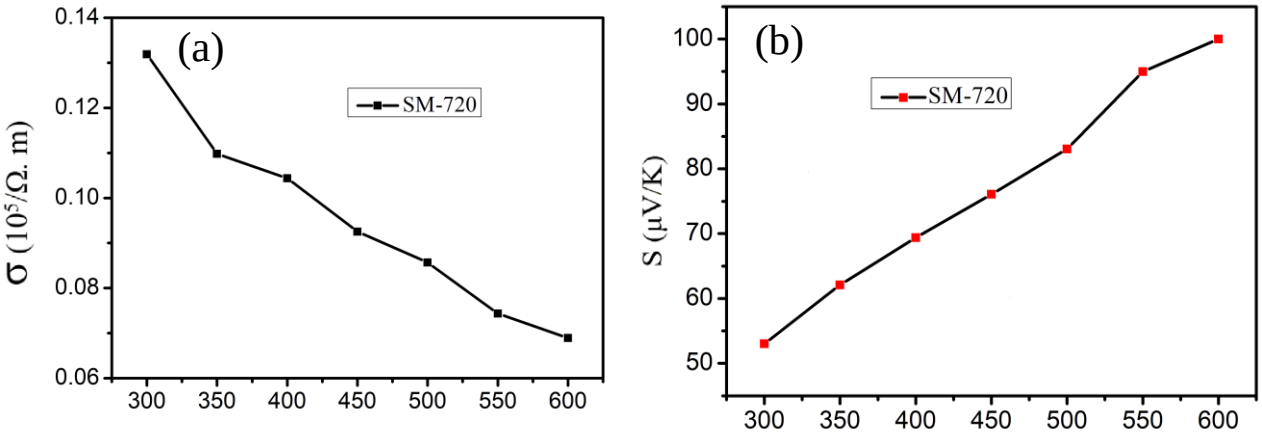


Figure S-5. Temperature dependence of (a) electrical conductivity and (b) Seebeck coefficient for the spark-plasma-sintered sample (SM-720).

Table S1. Chemical compositions of the samples M-720, M-820 and C-960 analyzed by inductively coupled plasma atomic emission spectroscopy (ICP-AES)

Sample	Nominal composition	Analyzed composition
M-720	Cu_2SnSe_3	$Cu_2Sn_{0.937}Se_{2.959}$
M-820	Cu_2SnSe_3	$Cu_2Sn_{0.961}Se_{2.962}$
C-960	Cu_2SnSe_3	$Cu_2Sn_{0.931}Se_{2.945}$

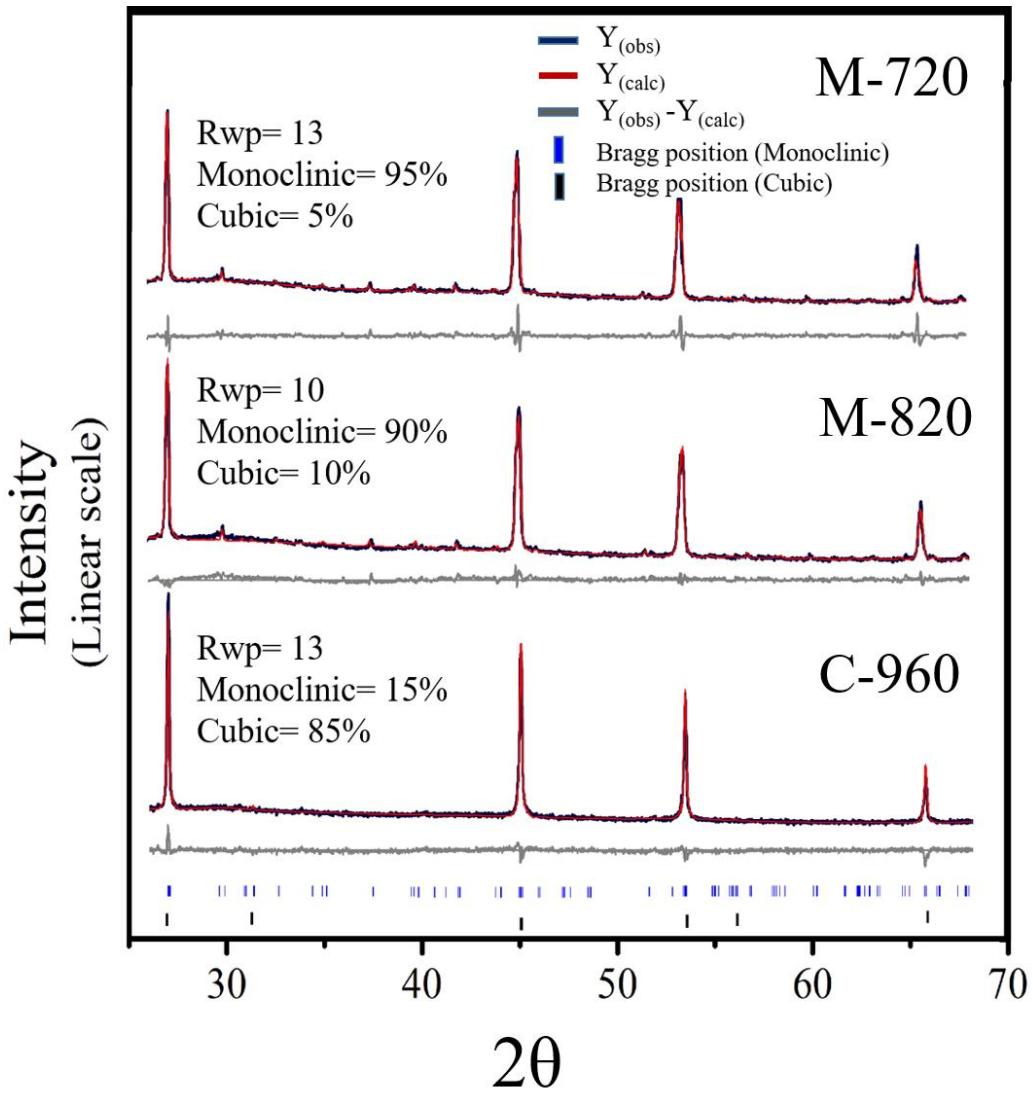


Fig S-6. Results of the Rietveld refinement quantitative phase analyses of M-720, M-820 and C-960 samples are shown along with Rwp values in the upper left corner of each pattern. The dark blue line is the original pattern; the red line is the calculated one; the grey line shows the difference between calculated and observed patterns; the blue and black dashed dots show the Bragg peak positions of the corresponding monoclinic and cubic phases.