Syntheses of a series of $BaCu_{2-x}Ag_xSe_2$ (x = 0 – 1.0) selenides and evaluation of their thermoelectric properties

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Electronic Supplementary Information (ESI)

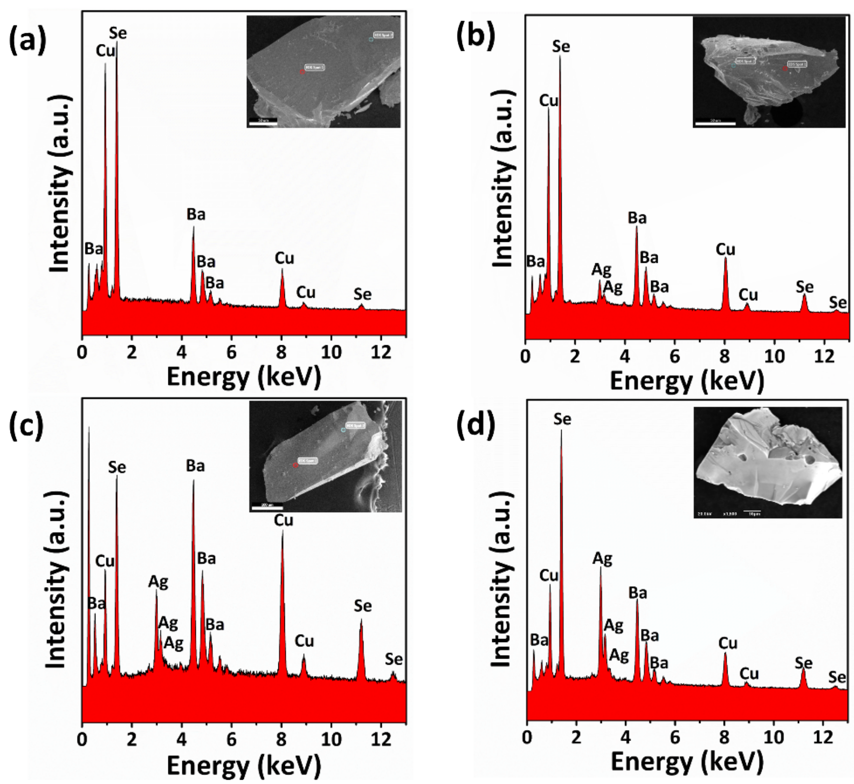

Fig. SI1: The EDX spectra collected for **(a)** the $x = 0$, **(b)** $x = 0.22$, **(c)** $x = 0.43$, and (d) $x = 0.8$ crystals used for single crystal X-ray diffraction studies.

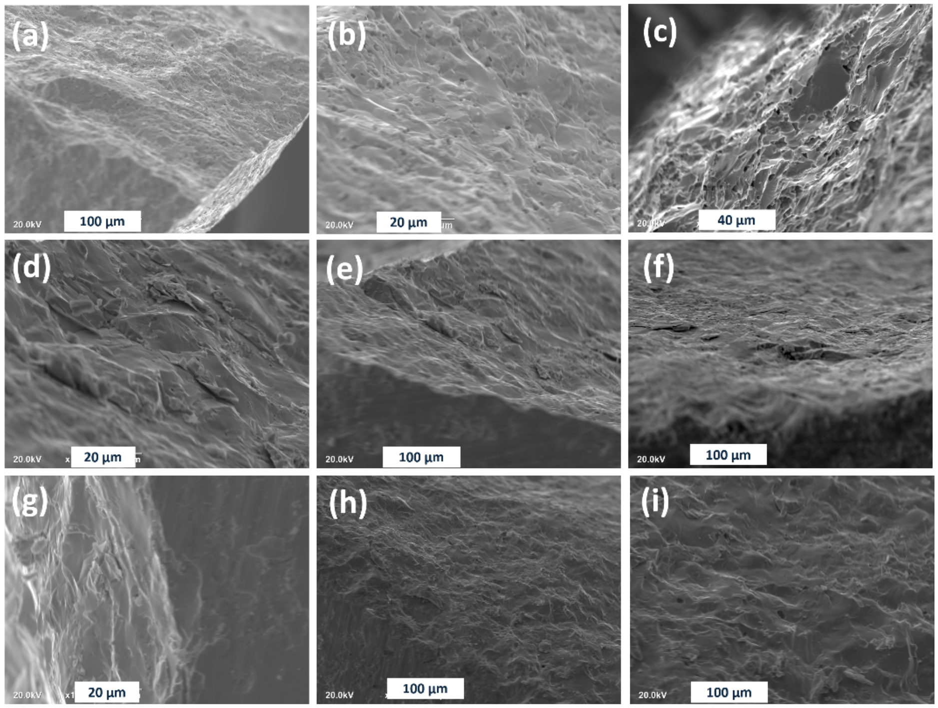

Fig. SI2: The SEM micrographs for the fractured surfaces of the pellets of **(a-c)** $BaCu_2Se_2$, **(d-f)** $BaCu_{1.5}Ag_{0.5}Se_2$, and **(g-i)** $BaCuAgSe_2$ samples after thermal conductivity studies.

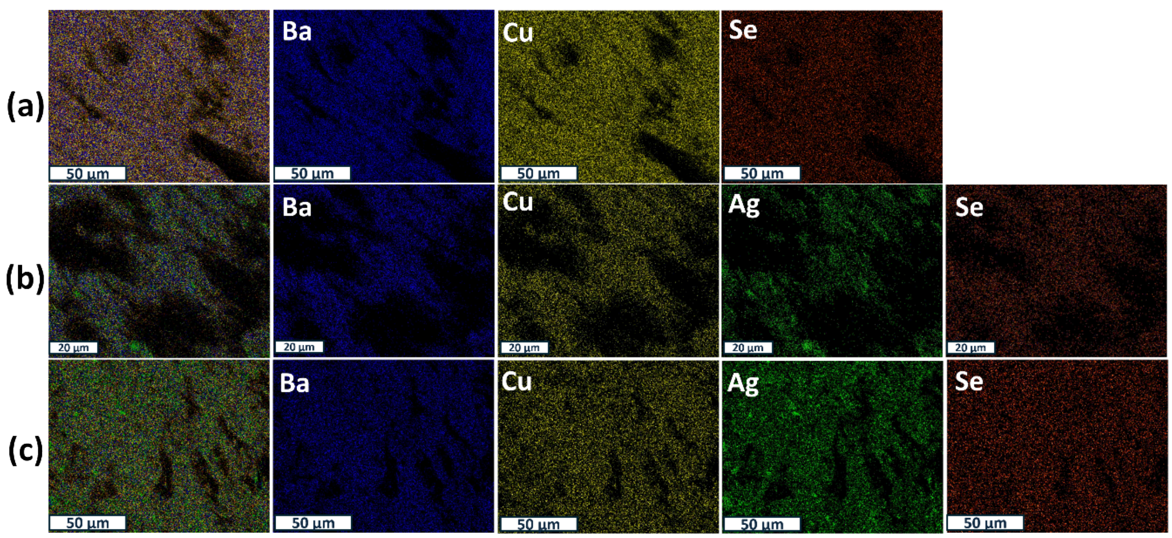

Fig. SI3: The EDX elemental mapping images for the pellets of **(a)** $BaCu_2Se_2$, **(b)** $BaCu_{1.5}Ag_{0.5}Se_2$, and **(c)** $BaCuAgSe_2$ samples after thermal conductivity measurements.

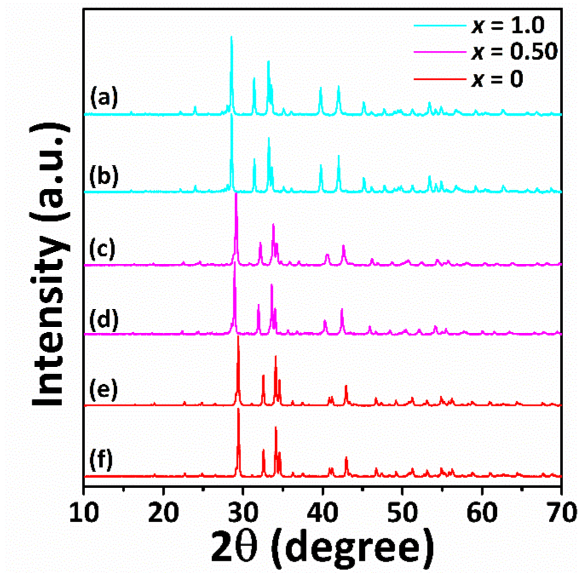

Fig. SI4: A comparison of the PXRD patterns for the polycrystalline $BaCu_2Se_2$, $BaCu_{0.5}Ag_{0.5}Se_2$, and $BaCuAgSe_2$ samples before and after thermal conductivity studies. The PXRD patterns marked with **(a)**, **(c)**, and **(e)** labels correspond to the patterns after the thermal conductivity studies, whereas **(b)**, **(d)**, and **(f)** are the patterns of as-synthesized samples shown for reference.

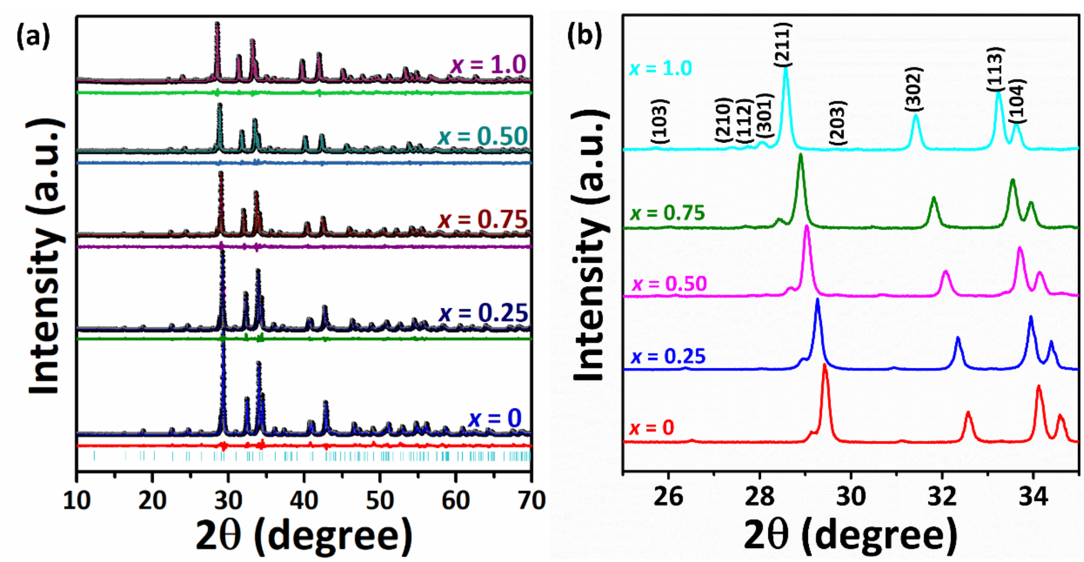

Fig. SI5: (a) The Le-Bail refinement plots of the PXRD patterns for the polycrystalline $BaCu_{2-x}Ag_xSe_2$ (x = 0, 0.25, 0.50, 0.75, and 1.0) samples at RT and **(b)** the PXRD patterns for the $BaCu_{2-x}Ag_xSe_2$ samples from 2θ range of 25° to 35° showing the peak shift with increase in the Ag concentration.

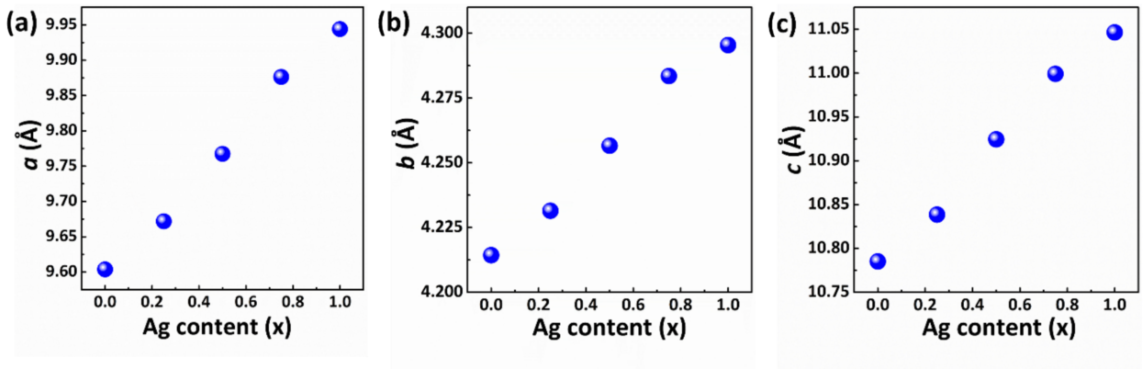

Fig. SI6: The refined unit cell parameters (Å) of the polycrystalline $BaCu_{2-x}Ag_xSe_2$ (x = 0, 0.25, 0.51, 0.75, 1.0) samples as a function of Ag content (x).

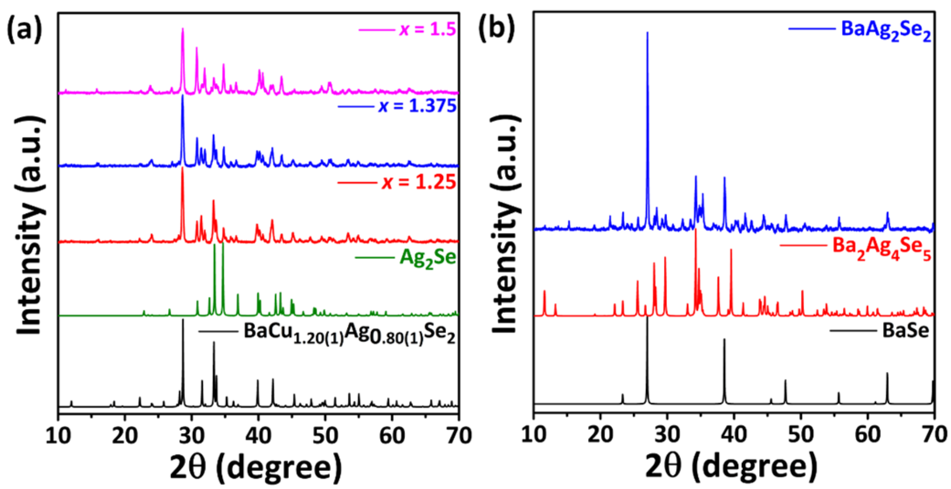

Fig. SI7: (a) The experimental PXRD patterns of the products of the reactions with the loaded compositions of $BaCu_{2-x}Ag_xSe_2$ (x = 1.25, 1.375, and 1.5) and **(b)** $BaAg_2Se_2$. These figures also contain theoretical PXRD patterns of the $BaCu_{1.20(1)}Ag_{0.80(1)}Se_2$, Ag_2Se,[1] BaSe,[2] and $Ba_2Ag_4Se_5$.[3]

Table SI1: The atomic displacement parameters (Å^2) for the $BaCu_{2-x}Ag_xSe_2$ (x = 0, 0.22, 0.43, 0.51, and 0.80) structures.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
$BaCu_2Se_2$						
Ba1	0.01194(18)	0.00785(17)	0.00872(18)	0.000	0.00063(12)	0.000
Cu1	0.0199(4)	0.0139(4)	0.0174(4)	0.000	0.0047(3)	0.000
Cu2	0.0144(4)	0.0202(4)	0.0158(4)	0.000	-0.0008(3)	0.000
Se1	0.0089(3)	0.0073(3)	0.0078(3)	0.000	0.0003(2)	0.000

Se2	0.0105(3)	0.0077(3)	0.0078(3)	0.000	0.0001(2)	0.000
$BaCu_{1.78(1)}Ag_{0.22(1)}Se_2$						
Ba1	0.0139(2)	0.0099(2)	0.0103(2)	0.000	0.00043(15)	0.000
Cu1/Ag1	0.0211(5)	0.0167(5)	0.0201(6)	0.000	0.0055(4)	0.000
Cu2/Ag2	0.0163(4)	0.0245(5)	0.0173(6)	0.000	-0.0013(3)	0.000
Se1	0.0140(3)	0.0120(3)	0.0096(4)	0.000	0.0007(3)	0.000
Se2	0.0129(3)	0.0126(3)	0.0138(4)	0.000	0.0012(3)	0.000
$BaCu_{1.57(1)}Ag_{0.43(1)}Se_2$						
Ba1	0.0174(2)	0.01122(19)	0.01131(19)	0.000	0.00063(12)	0.000
Cu1/Ag1	0.0247(4)	0.0184(4)	0.0236(4)	0.000	0.0056(3)	0.000
Cu2/Ag2	0.0192(4)	0.0256(4)	0.0185(4)	0.000	-0.0015(3)	0.000
Se1	0.0201(3)	0.0151(3)	0.0108(3)	0.000	0.0014(2)	0.000
Se2	0.0162(3)	0.0139(3)	0.0175(3)	0.000	0.0023(2)	0.000
$BaCu_{1.49(1)}Ag_{0.51(1)}Se_2$						
Ba1	0.01623(13)	0.00841(12)	0.01028(13)	0.000	0.00054(7)	0.000
Cu1/Ag1	0.0235(3)	0.0164(3)	0.0232(3)	0.000	0.00573(19)	0.000
Cu2/Ag2	0.0179(2)	0.0221(3)	0.0173(3)	0.000	-0.00128(16)	0.000
Se1	0.0193(2)	0.01296(19)	0.0097(2)	0.000	0.00131(14)	0.000
Se2	0.01538(19)	0.01168(19)	0.0178(2)	0.000	0.00276(14)	0.000
$BaCu_{1.20(1)}Ag_{0.80(1)}Se_2$						
Ba1	0.01624(17)	0.01166(17)	0.01071(17)	0.000	0.00025(12)	0.000
Cu1/Ag1	0.0237(4)	0.0206(4)	0.0239(4)	0.000	0.0056(3)	0.000
Cu2/Ag2	0.0185(3)	0.0248(3)	0.0188(3)	0.000	-0.0017(2)	0.000
Se1	0.0204(3)	0.0182(3)	0.0108(3)	0.000	0.0016(2)	0.000
Se2	0.0170(3)	0.0159(3)	0.0196(3)	0.000	0.0037(2)	0.000

References

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