Supplementary materials

Stabilized cubic phase $BiAgSe_{2-x}S_x$ with excellent thermoelectric properties *via* phase boundary engineering

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Table S1 Densities of $BiAgSe_{2-x}S_x$ (x = 0.8 - 1.2).

Composition	Theoretical Density (g/cm³)	Measured Density (g/cm³)	Relative Density (%)
$BiAgSe_{1.2}S_{0.8}$	7.79	7.23	92.81
$BiAgSe_{1.1}S_{0.9}$	7.67	7.45	97.13
$BiAgSeS$	7.52	7.47	99.34
$BiAgSe_{0.9}S_{1.1}$	7.42	7.39	99.60
$BiAgSe_{0.8}S_{1.2}$	7.29	7.14	97.94
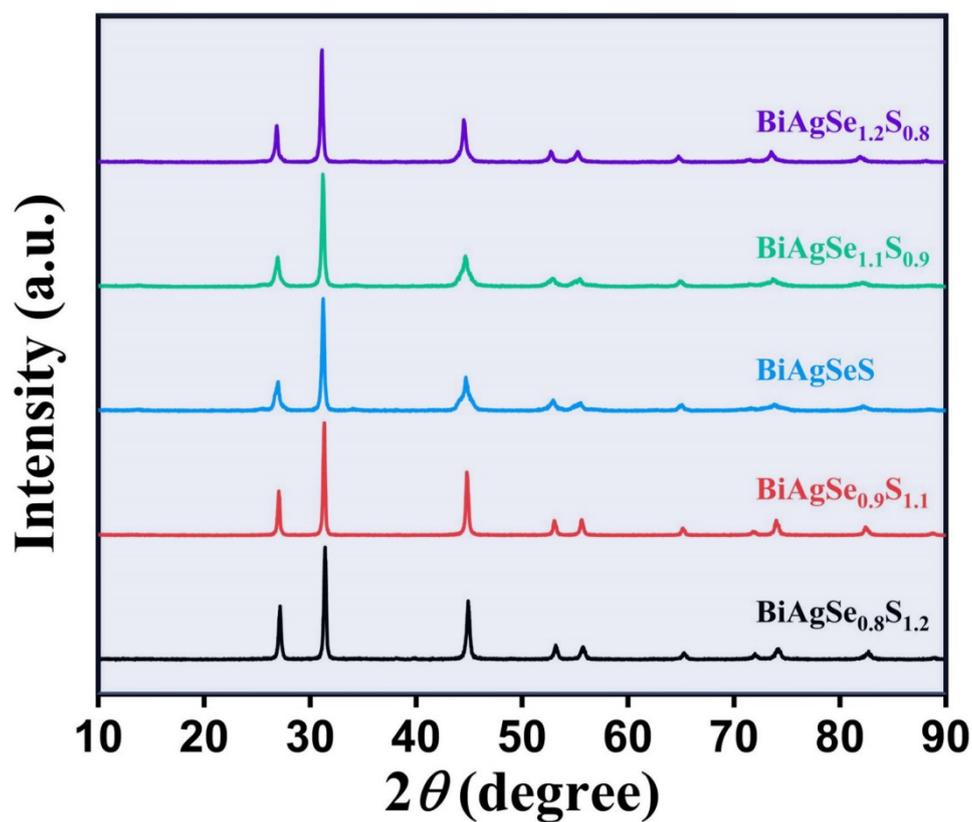
Fig. S1 Powder XRD patterns for $BiAgSe_{2-x}S_x$ (x = 0.8 - 1.2) before heating-cooling cycle (HCC). All the samples crystalline in cubic structure.
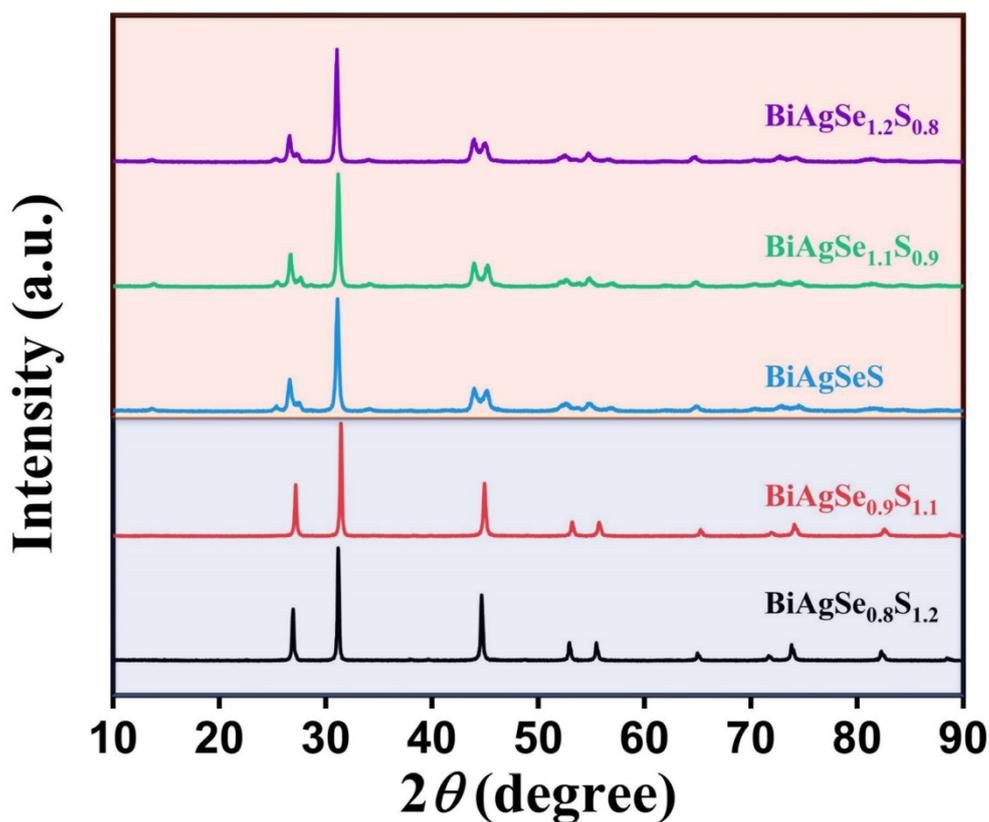
Fig. S2 Powder XRD patterns for $BiAgSe_{2-x}S_x$ (x = 0.8 - 1.2) after one heating-cooling cycle (HCC). Only $BiAgSe_{0.9}S_{1.1}$ and $BiAgSe_{0.8}S_{1.2}$ were still cubic phase.
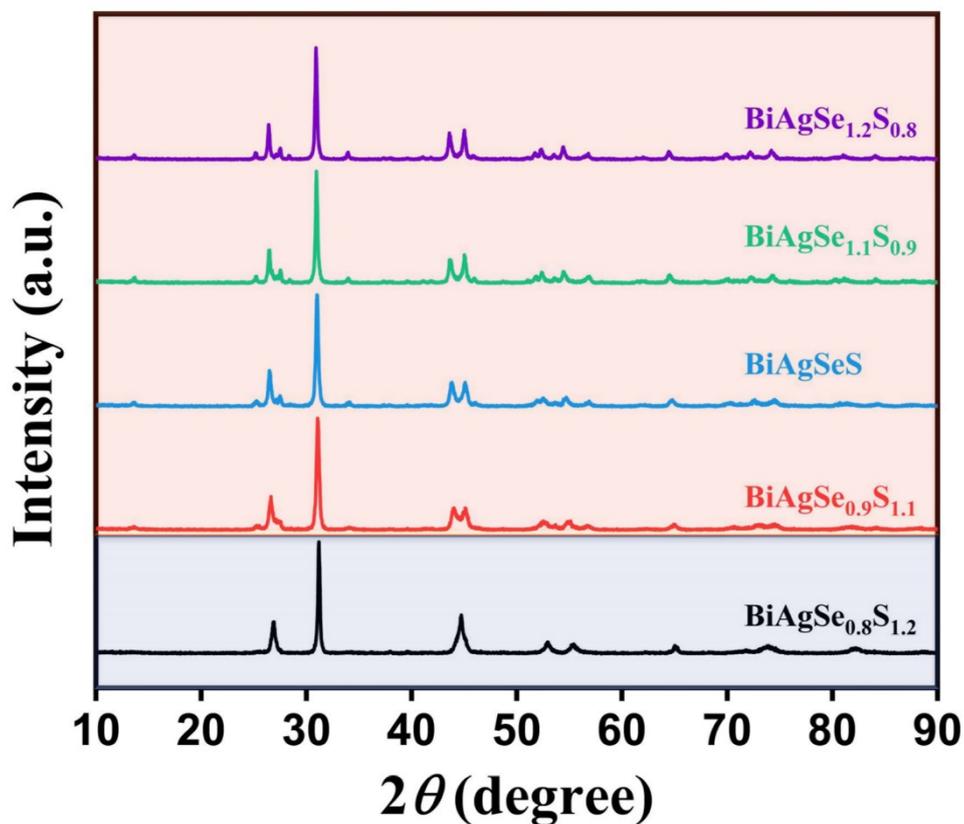
Fig. S3 Powder XRD patterns for $BiAgSe_{2-x}S_x$ (x = 0.8 - 1.2) after two heating-cooling cycle (HCC). Only $BiAgSe_{0.8}S_{1.2}$ was still cubic phase.
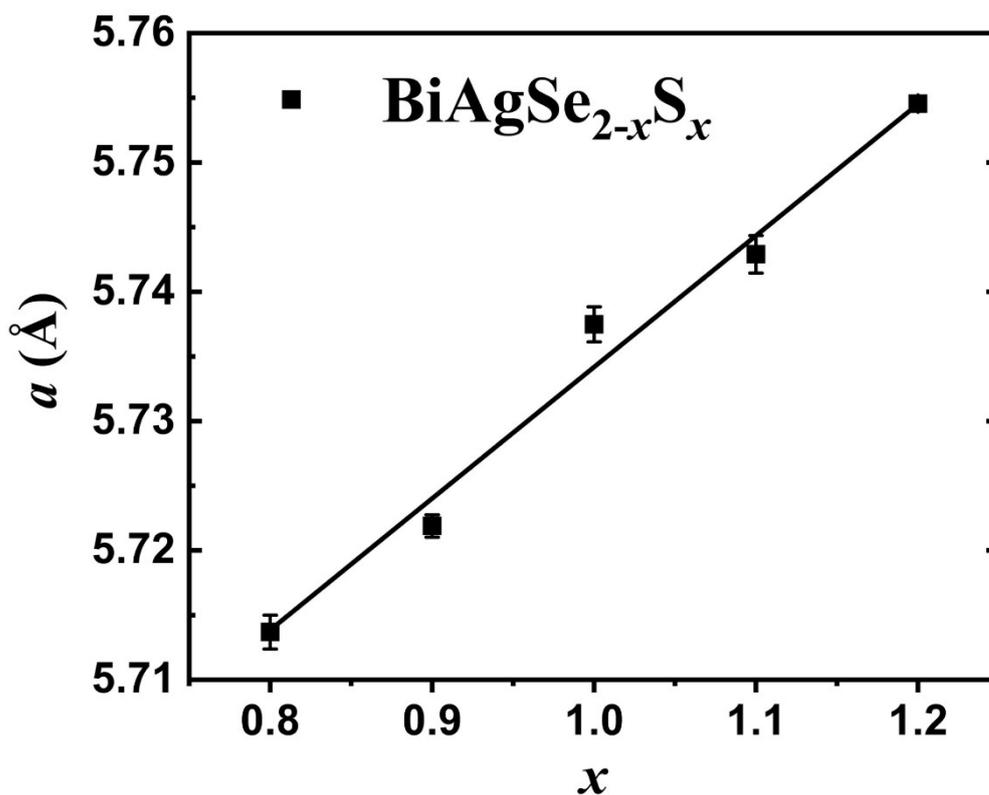
Fig. S4 Lattice parameters of BiAgSe$_{2-x}$S$_x$ (x = 0.8 - 1.2) before heating-cooling cycle, which fit the Vegard's law well.
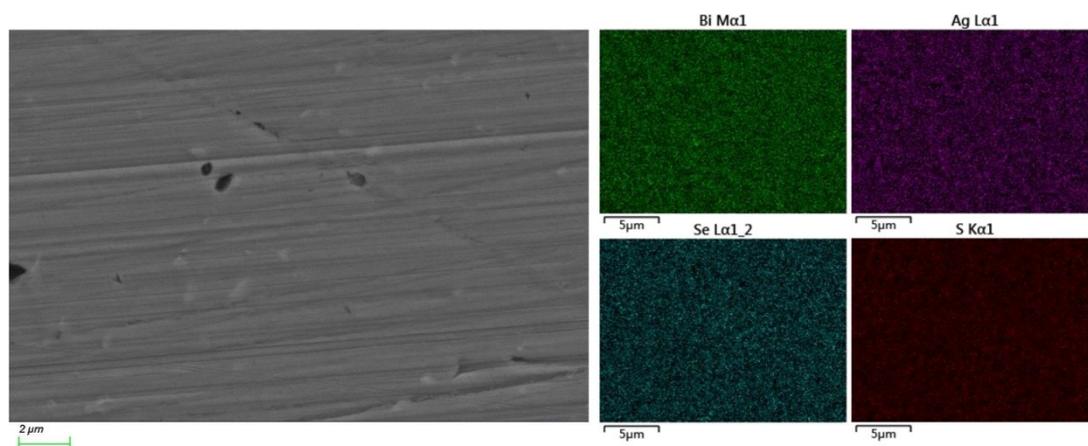
Element	Atomic%	Normalization
S	27.98	1.02
Se	19.57	0.71
Ag	27.55	1.00
Bi	24.90	0.90
Total	100.00	/

Fig. S5 EDS analysis of BiAgSe$_{0.8}$S$_{1.2}$.
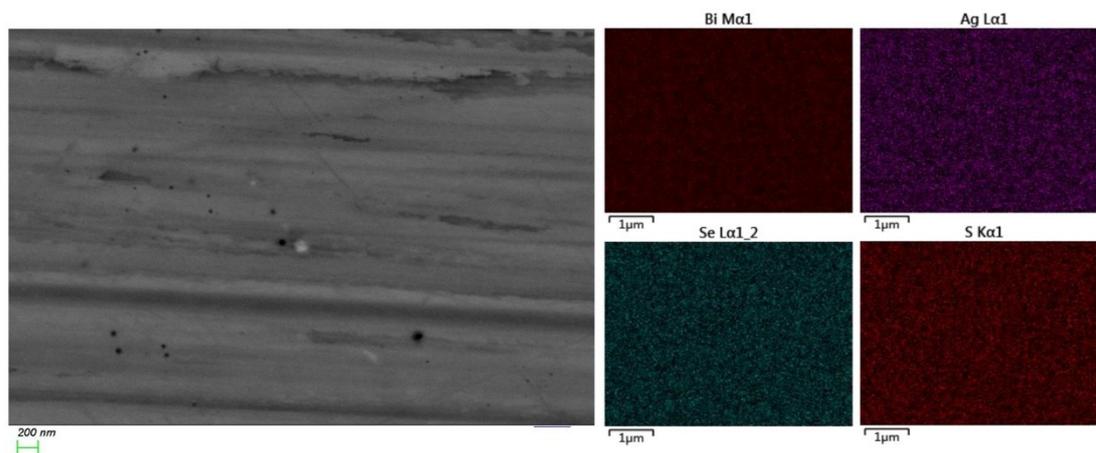
Element	Atomic%	Normalization
S	23.71	0.90
Se	24.55	0.93
Ag	26.49	1.00
Bi	25.25	0.95
Total	100.00	/

Fig. S6 EDS analysis of BiAgSeS.
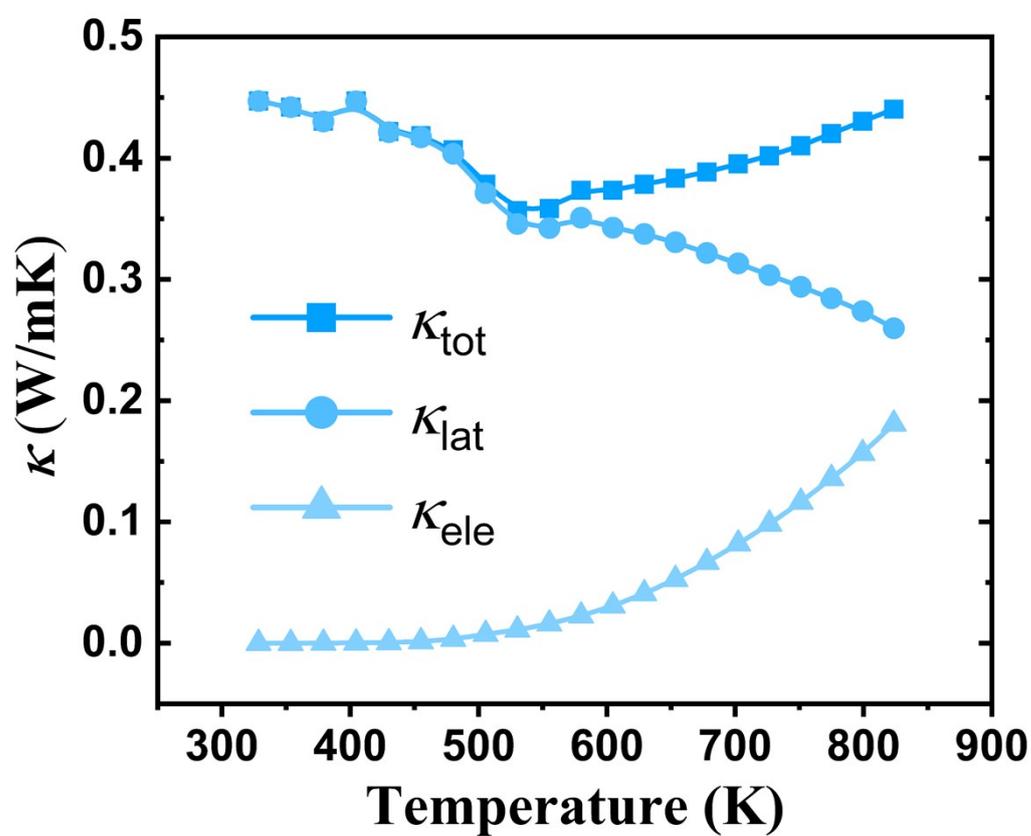
Fig. S7 Temperature-dependent total thermal conductivity, lattice thermal conductivity and electronic thermal conductivity of BiAgSe$_{0.8}$S$_{1.2}$.
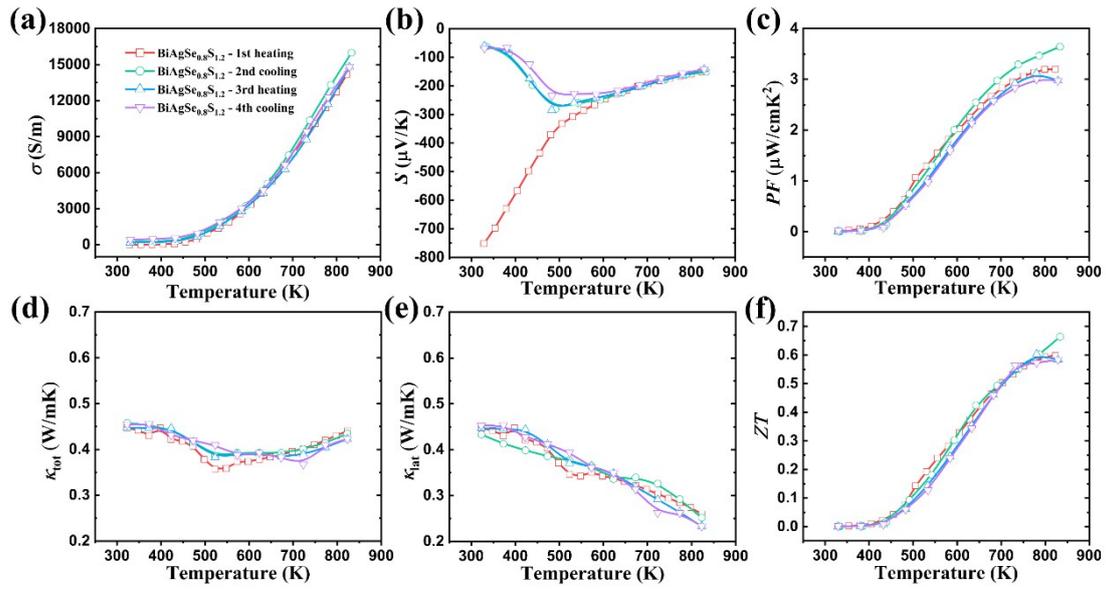
Fig. S8 Repeatedly measured temperature-dependence of (a) electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) total thermal conductivity, (e) lattice thermal conductivity and (f) ZT for cubic BiAgSe$_{0.8}$S$_{1.2}$.