Supporting Information

Compound Defects and Thermoelectric Properties in Ternary CuAgSe-based Materials

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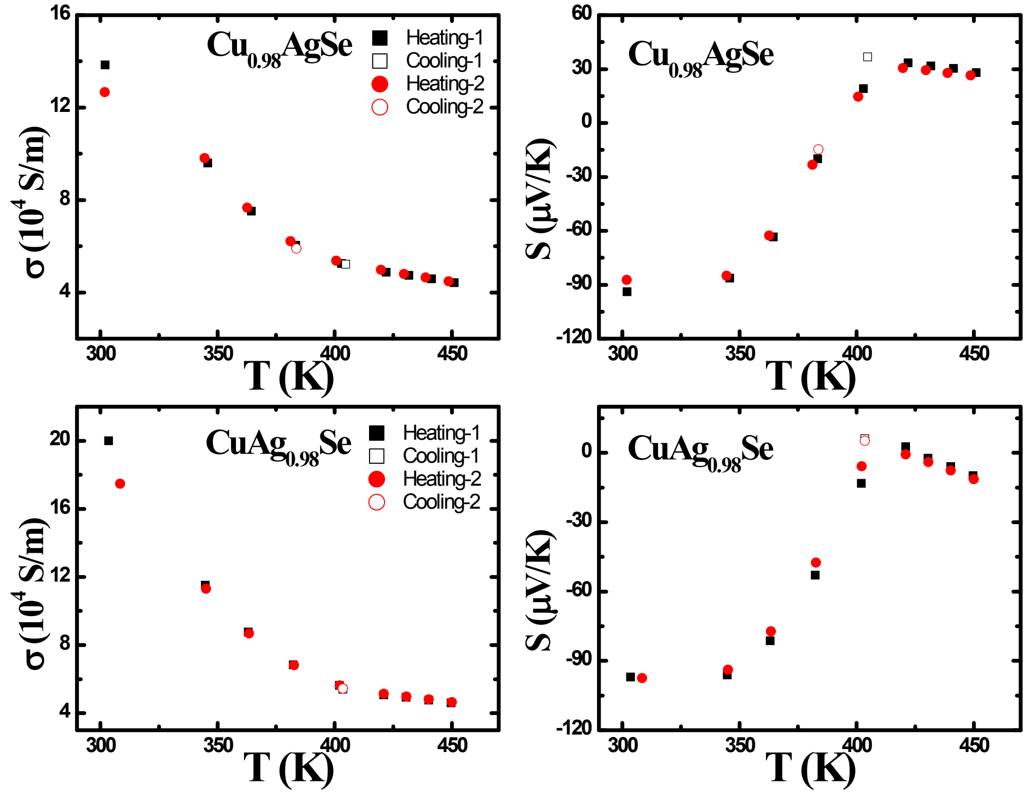

Fig. S1 Cycle measurements of electrical conductivity σ and thermopower S from 300 K to 450 K for sample $Cu_{0.98}AgSe$ and $CuAg_{0.98}Se$.

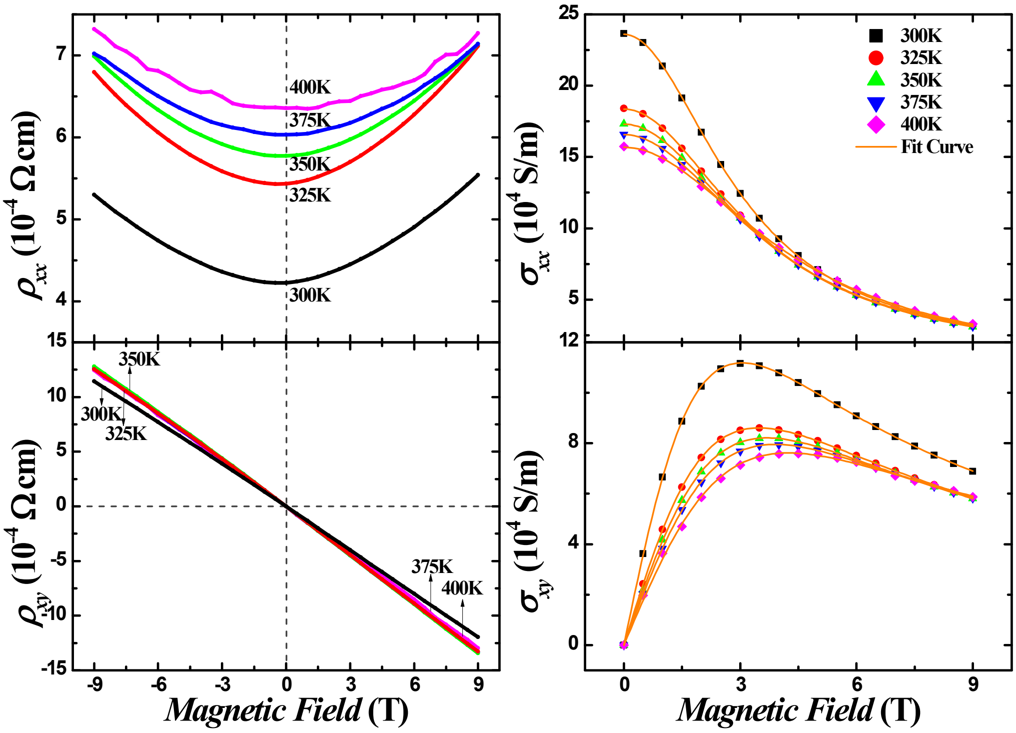

Fig. S2 Magnetic field dependence of longitudinal electrical resistivity ρ_{xx} (a) and Hall resistivity ρ_{xy} (b) of β-CuAgSe from 300 K to 400 K, and the calculated longitudinal conductivity σ_{xx} (c) and Hall conductivity σ_{xy} (d). The solid lines in (c) and (d) are the fits using Equation (3) and (4).

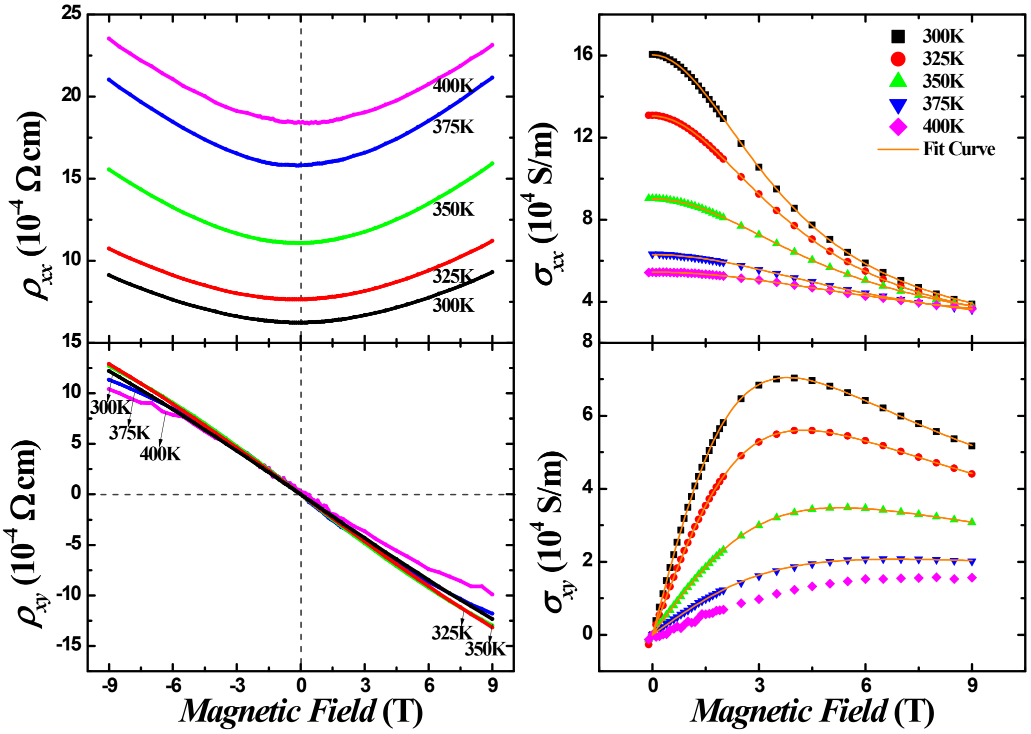

Fig. S3 Magnetic field dependence of longitudinal electrical resistivity ρ_{xx} (a) and Hall resistivity ρ_{xy} (b) of $Cu_{0.99}AgSe$ from 300 K to 400 K, and the calculated longitudinal conductivity σ_{xx} (c) and Hall conductivity σ_{xy} (d). The solid lines in (c) and (d) are the fits using Equation (3) and (4).

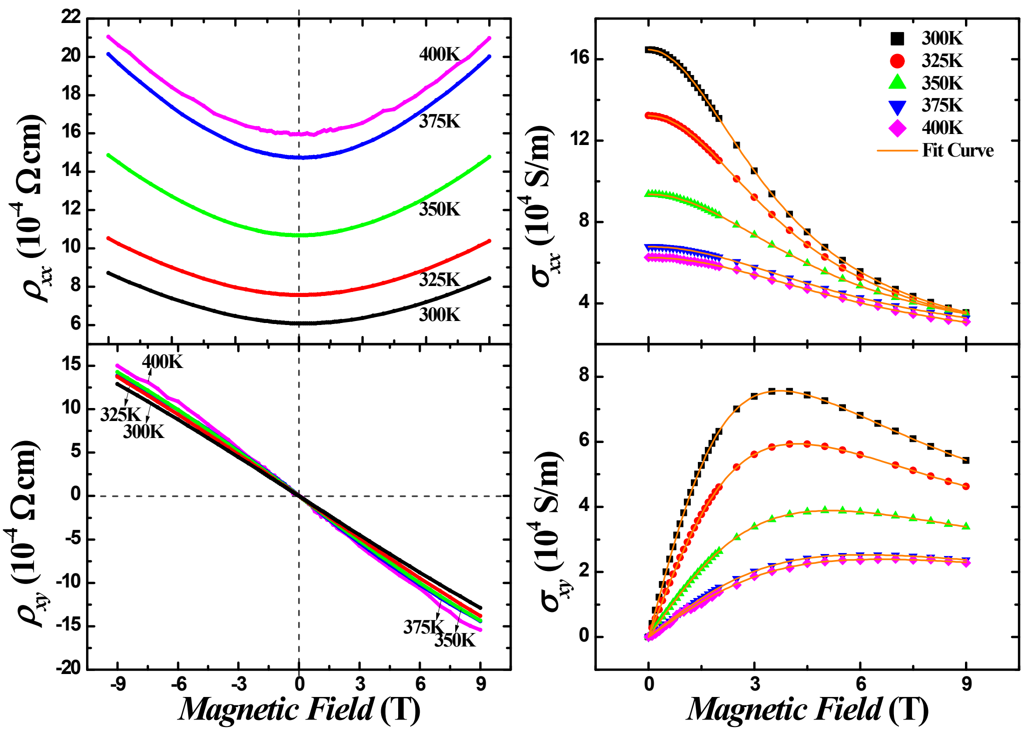

Fig. S4 Magnetic field dependence of longitudinal electrical resistivity ρ_{xx} (a) and Hall resistivity ρ_{xy} (b) of $CuAg_{0.99}Se$ from 300 K to 400 K, and the calculated longitudinal conductivity σ_{xx} (c) and Hall conductivity σ_{xy} (d). The solid lines in (c) and (d) are the fits using Equation (3) and (4).

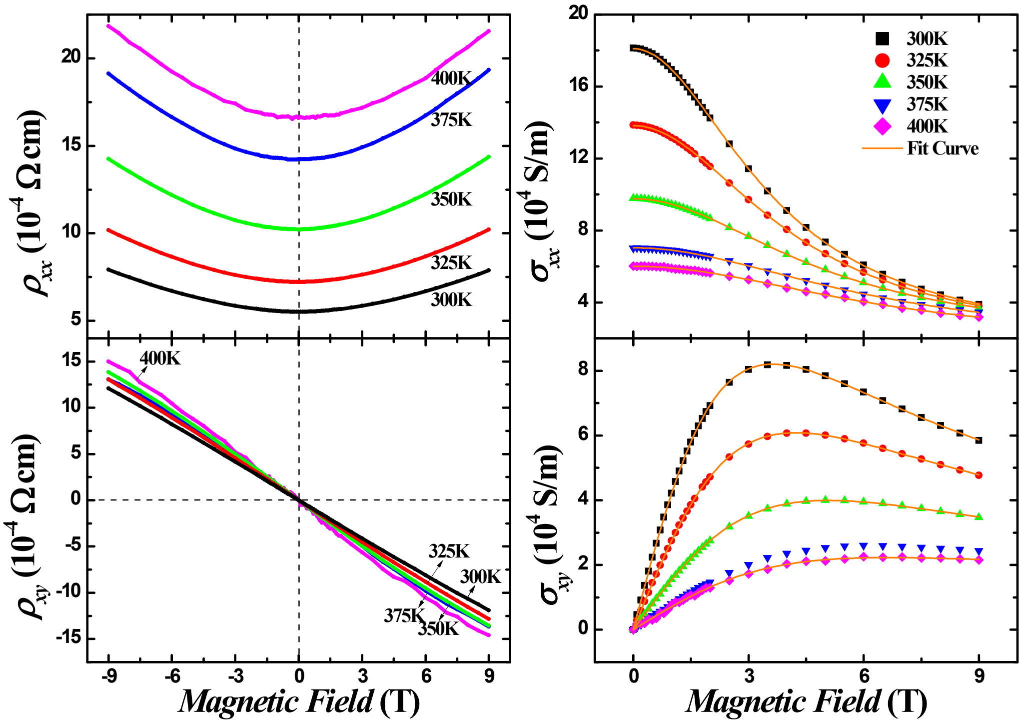

Fig. S5 Magnetic field dependence of longitudinal electrical resistivity ρ_{xx} (a) and Hall resistivity ρ_{xy} (b) of $CuAg_{0.98}Se$ from 300 K to 400 K, and the calculated longitudinal conductivity σ_{xx} (c) and Hall conductivity σ_{xy} (d). The solid lines in (c) and (d) are the fits using Equation (3) and (4).

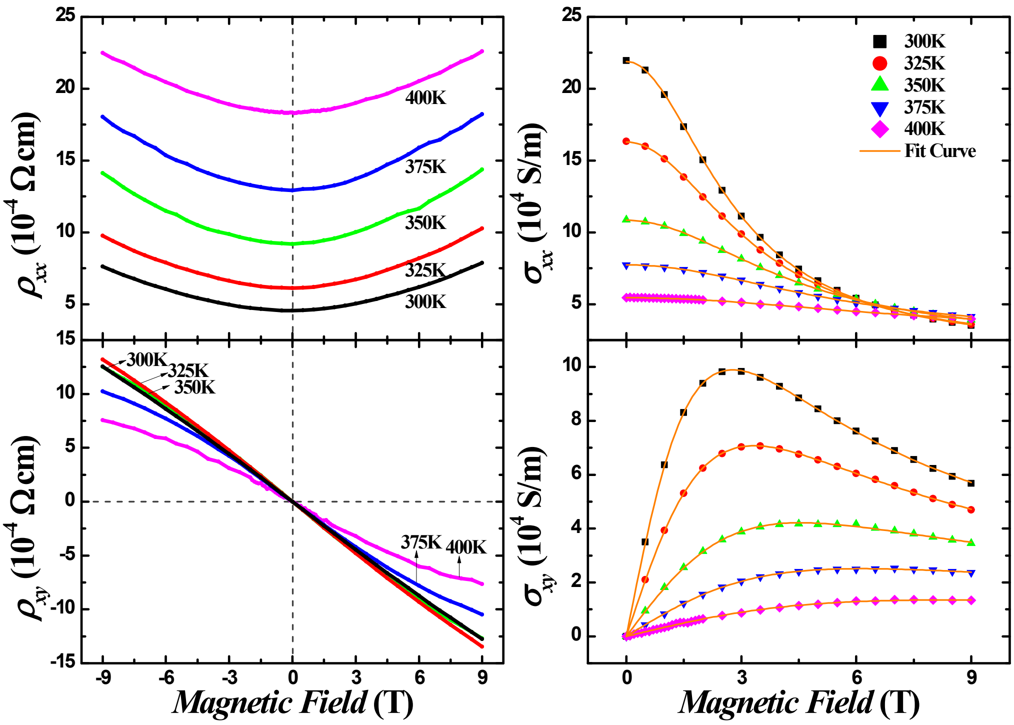

Fig. S6 Magnetic field dependence of longitudinal electrical resistivity ρ_{xx} (a) and Hall resistivity ρ_{xy} (b) of $CuAgSe_{1.04}$ from 300 K to 400 K, and the calculated longitudinal conductivity σ_{xx} (c) and Hall conductivity σ_{xy} (d). The solid lines in (c) and (d) are the fits by using Equation (3) and (4).

Fig. S7 Ingot samples after high temperature annealing. $CuAg_{1.01}Se$, $Cu_{1.01}AgSe$, and $CuAgSe_{0.99}$ display the same phenomenon as the left sample with the metallic Ag on the surface. The samples in the Section of 3.1.1-3.1.4 are the right one without obvious metallic Ag observed.

Table S1. Fitting parameters for sample β-CuAgSe.

T(K)	$n_{xx}(10^{18}\ cm^{-3})$	$\mu_{xx}(10^4\ cm^2/V\text{-}s)$	$C_{xx}(\Omega^{-1}m^{-1})$	$n_{xy}(10^{18}\ cm^{-3})$	$\mu_{xy}(10^4\ cm^2/V\text{-}s)$	$C_{xy}(10^{-3})$
300	4.32	0.33	8914.24	4.21	0.33	2.57
325	3.80	0.29	8811.22	3.72	0.29	2.25
350	3.85	0.27	6830.86	3.76	0.27	1.80
375	3.88	0.26	6057.52	3.84	0.26	1.94
400	4.17	0.23	3654.34	3.99	0.24	2.31

Table S2. Fitting parameters for sample $Cu_{0.99}AgSe$.

T(K)	$n_{xx}(10^{18}\ cm^{-3})$	$\mu_{xx}(10^4\ cm^2/V\text{-}s)$	$C_{xx}(\Omega^{-1}m^{-1})$	$n_{xy}(10^{18}\ cm^{-3})$	$\mu_{xy}(10^4\ cm^2/V\text{-}s)$	$C_{xy}(10^{-3})$
300	3.38	0.26	17837.22	3.25	0.27	7.84
325	2.96	0.24	17564.74	2.87	0.24	9.18
350	2.25	0.19	20613.82	2.15	0.20	15.83
375	1.62	0.16	22539.92	1.17	0.18	87.57

Table S3. Fitting parameters for sample $Cu_{0.98}AgSe$.

T(K)	$n_{xx}(10^{18}\ cm^{-3})$	$\mu_{xx}(10^4\ cm^2/V\text{-}s)$	$C_{xx}(\Omega^{-1}m^{-1})$	$n_{xy}(10^{18}\ cm^{-3})$	$\mu_{xy}(10^4\ cm^2/V\text{-}s)$	$C_{xy}(10^{-3})$
300	3.39	0.24	17126.60	3.27	0.24	5.93
325	2.67	0.20	18887.09	2.55	0.20	6.28
350	2.02	0.17	20636.09	1.86	0.17	4.92
375	1.48	0.14	22236.39	1.22	0.15	21.14
400	1.12	0.12	24620.52	0.80	0.13	62.87

Table S4. Fitting parameters for sample $CuAg_{0.99}Se$.

T(K)	n_{xx}(10^{18} cm^{-3})	μ_{xx}(10^4 cm^2/V-s)	C_{xx}($\Omega^{-1}m^{-1}$)	n_{xy}(10^{18} cm^{-3})	μ_{xy}(10^4 cm^2/V-s)	C_{xy}(10^{-3})
300	3.51	0.27	13629.32	3.44	0.27	5.29
325	3.10	0.24	13767.59	3.04	0.24	6.52
350	2.46	0.20	16103.31	2.39	0.20	11.16
375	1.91	0.17	17245.32	1.77	0.17	21.99
400	1.97	0.15	14044.87	1.68	0.17	36.66

Table S5. Fitting parameters for sample $CuAg_{0.98}Se$.

T(K)	n_{xx}(10^{18} cm^{-3})	μ_{xx}(10^4 cm^2/V-s)	C_{xx}($\Omega^{-1}m^{-1}$)	n_{xy}(10^{18} cm^{-3})	μ_{xy}(10^4 cm^2/V-s)	C_{xy}(10^{-3})
300	3.75	0.27	16023.47	3.63	0.28	7.35
325	3.20	0.24	16409.91	3.09	0.24	9.71
350	2.47	0.20	18383.47	2.37	0.20	16.60
400	1.78	0.15	16628.66	1.37	0.18	67.87

Table S6. Fitting parameters for sample $CuAgSe_{1.04}$.

T(K)	n_{xx}(10^{18} cm^{-3})	μ_{xx}(10^4 cm^2/V-s)	C_{xx}($\Omega^{-1}m^{-1}$)	n_{xy}(10^{18} cm^{-3})	μ_{xy}(10^4 cm^2/V-s)	C_{xy}(10^{-3})
300	3.50	0.36	17979.08	3.38	0.36	3.44
325	3.02	0.30	18668.98	2.89	0.30	5.10
350	2.37	0.23	22767.92	2.24	0.23	16.11
375	1.83	0.17	26563.32	1.56	0.18	48.51
400	1.25	0.13	28859.85	1.15	0.13	47.33