Supplementary Materials

$Cu_{2-x}S$ and $Cu_{2-x}Se$ Alloys: Investigating the Influence of Ag, Zn, and Ni Doping on Structure and Transport Behavior

Andrzej Mikuła *, Tomasz Kurek, Miłosz Kożusznik and Paweł Nieroda

* Correspondence: amikula@agh.edu.pl

Table S1. Density of copper (I) chalcogenide sinters.

Material	Density [g cm^{-1}]	Material	Density [g cm^{-1}]
$Cu_{1.97}S$	5.51	$Cu_{1.8}Se$	6.10
$Cu_{1.96}Ag_{0.01}S$	5.37	$Cu_{1.79}Ag_{0.01}Se$	6.13
$Cu_{1.96}Ni_{0.01}S$	5.54	$Cu_{1.79}Ni_{0.01}Se$	6.06
$Cu_{1.96}Zn_{0.01}S$	5.49	$Cu_{1.79}Zn_{0.01}Se$	6.04

Table S2. Unit cell parameters together with fitting parameters for $Cu_{1.97}S$ and $Cu_{1.8}Se$ sintered pellets.

Structural parameter	This work	Reference card	GoF [–]	wRp [–]
$Cu_{1.97}S$ – Reference card Cu_2S (ICDD 01-083-1462)				
a [Å]	15.229	15.246	3.26	14.31
b [Å]	11.882	11.884		
c [Å]	13.495	13.494		
β [°]	116.266	116.350		
$Cu_{1.8}Se$ – Reference card (ICSD 98-015-0759)				
a [Å]	5.754	5.750	3.72	8.10

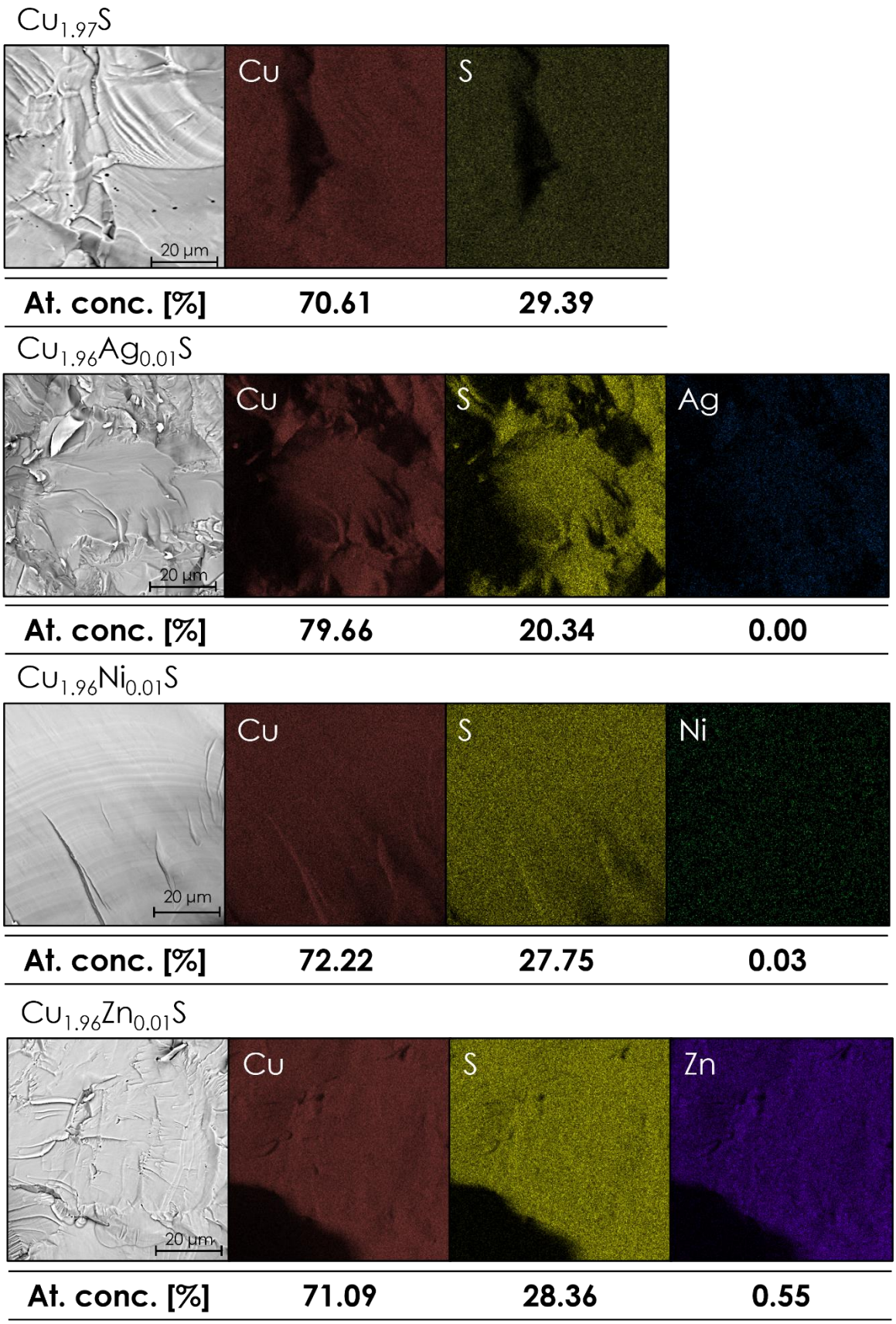


Figure S1. SEM+EDX analysis of $Cu_{1.97-x}M_xS$ (M = Ag, Ni, Zn; x = 0, 0.01) ingots.

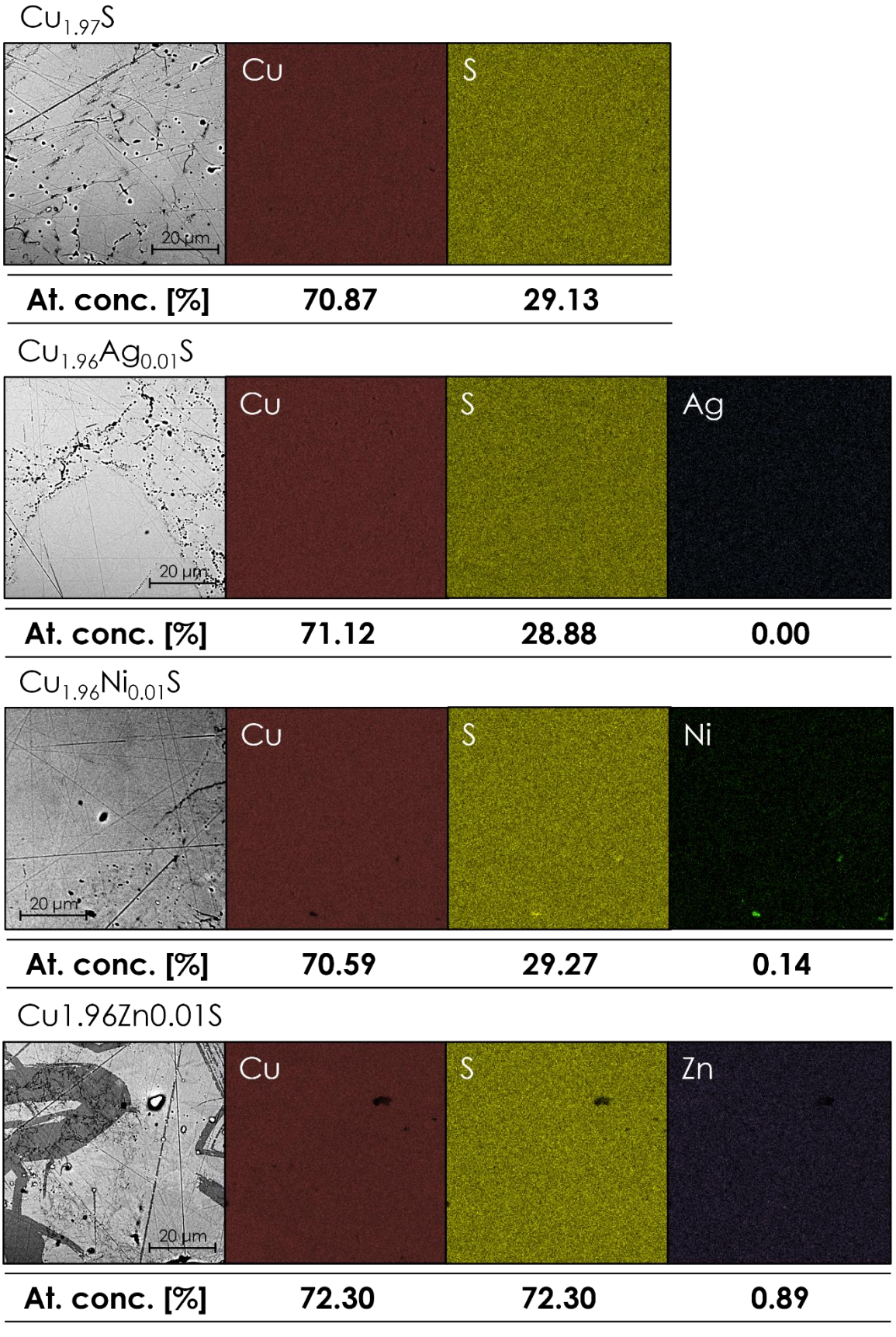


Figure S2. SEM+EDX analysis of $Cu_{1.97-x}M_xS$ (M = Ag, Ni, Zn; x = 0, 0.01) pellets.

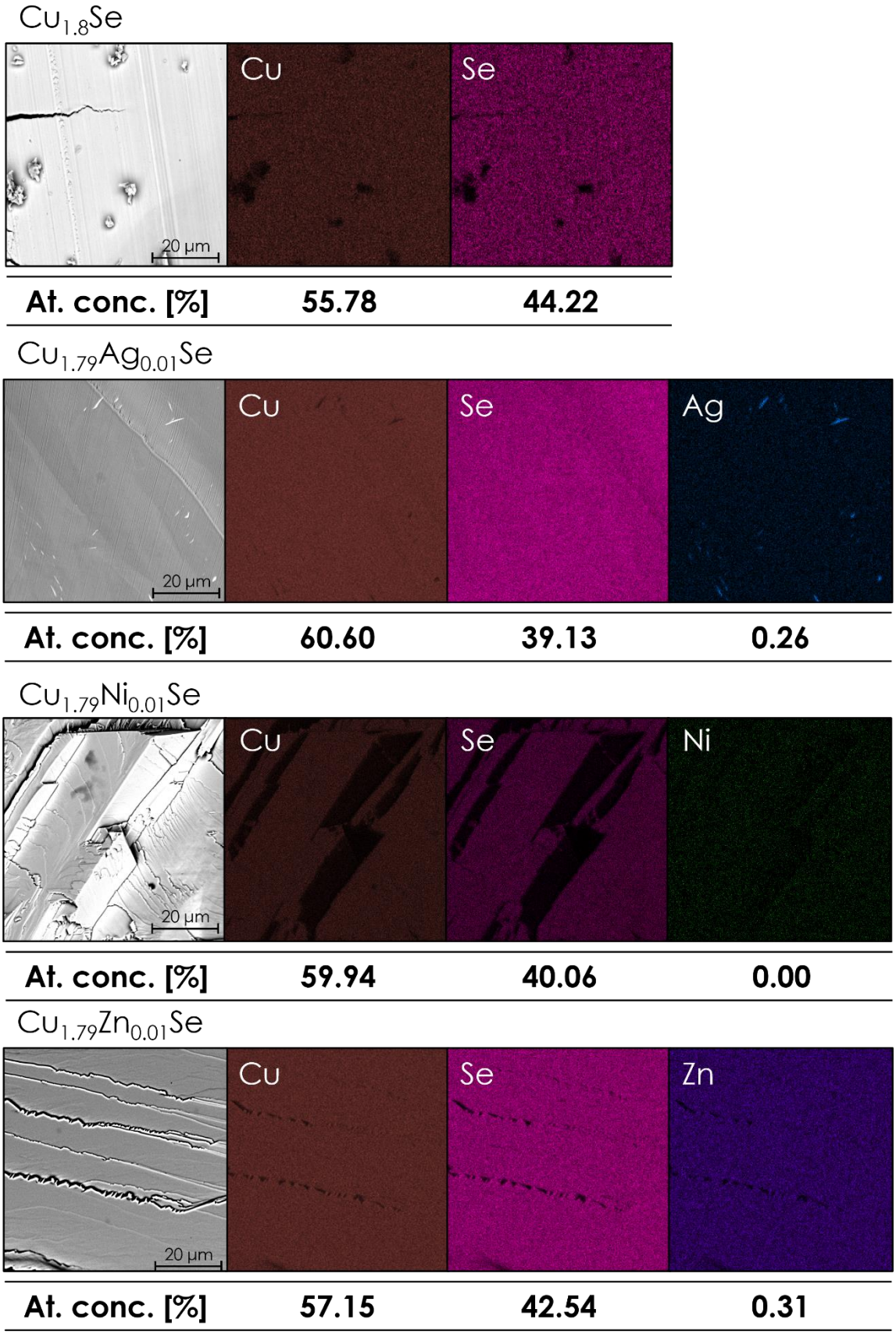
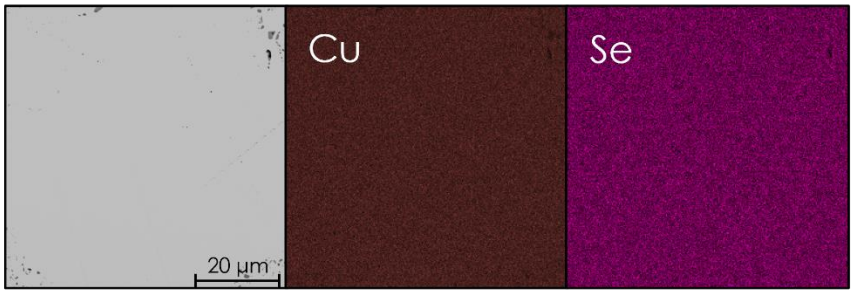


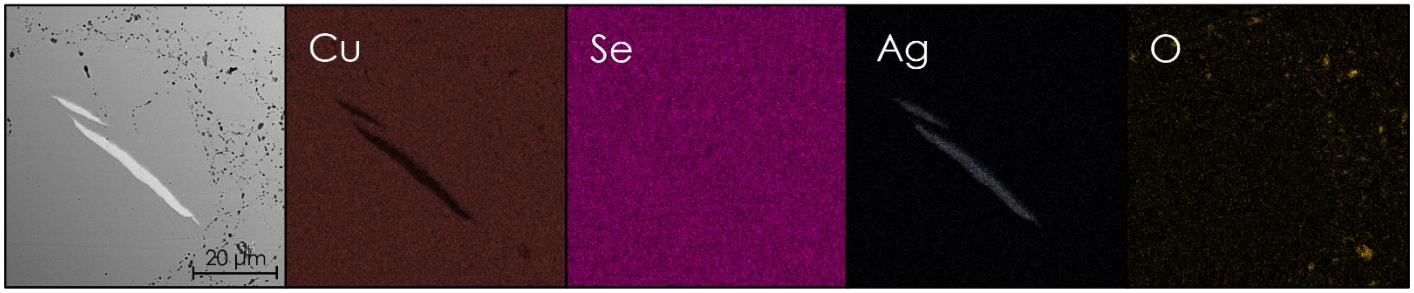
Figure S3. SEM+EDX analysis of $Cu_{1.8-x}M_xSe$ (M = Ag, Ni, Zn; x = 0, 0.01) ingots.

$Cu_{1.8}Se$



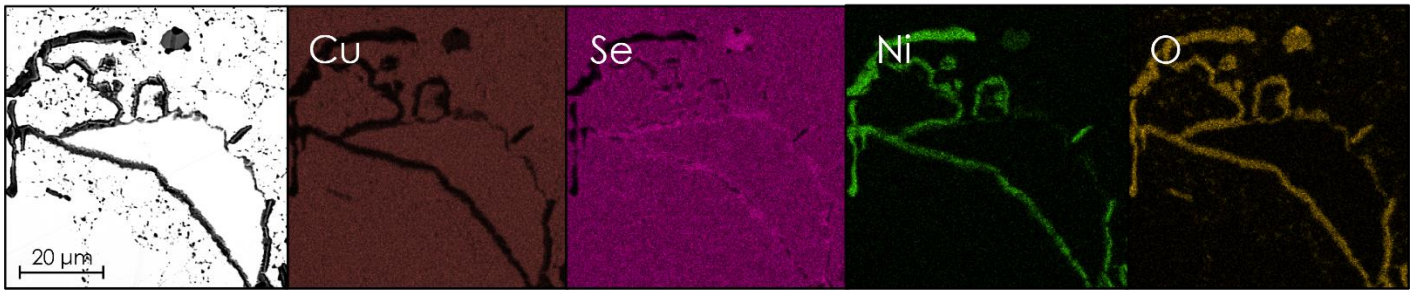
At. conc. [%]	59.17	40.83

$Cu_{1.79}Ag_{0.01}Se$



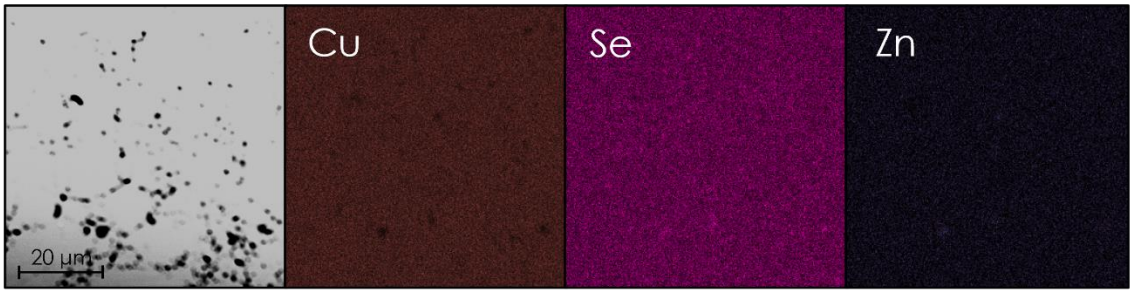
At. conc. [%]	55.61	39.99	1.17	3.32

$Cu_{1.79}Ni_{0.01}Se$



At. conc. [%]	46.97	35.60	4.74	12.69

$Cu_{1.79}Zn_{0.01}Se$



At. conc. [%]	58.25	41.31	0.44

Figure S4. SEM+EDX analysis of $Cu_{1.8-x}M_xSe$ (M = Ag, Ni, Zn; x = 0, 0.01) pellets.

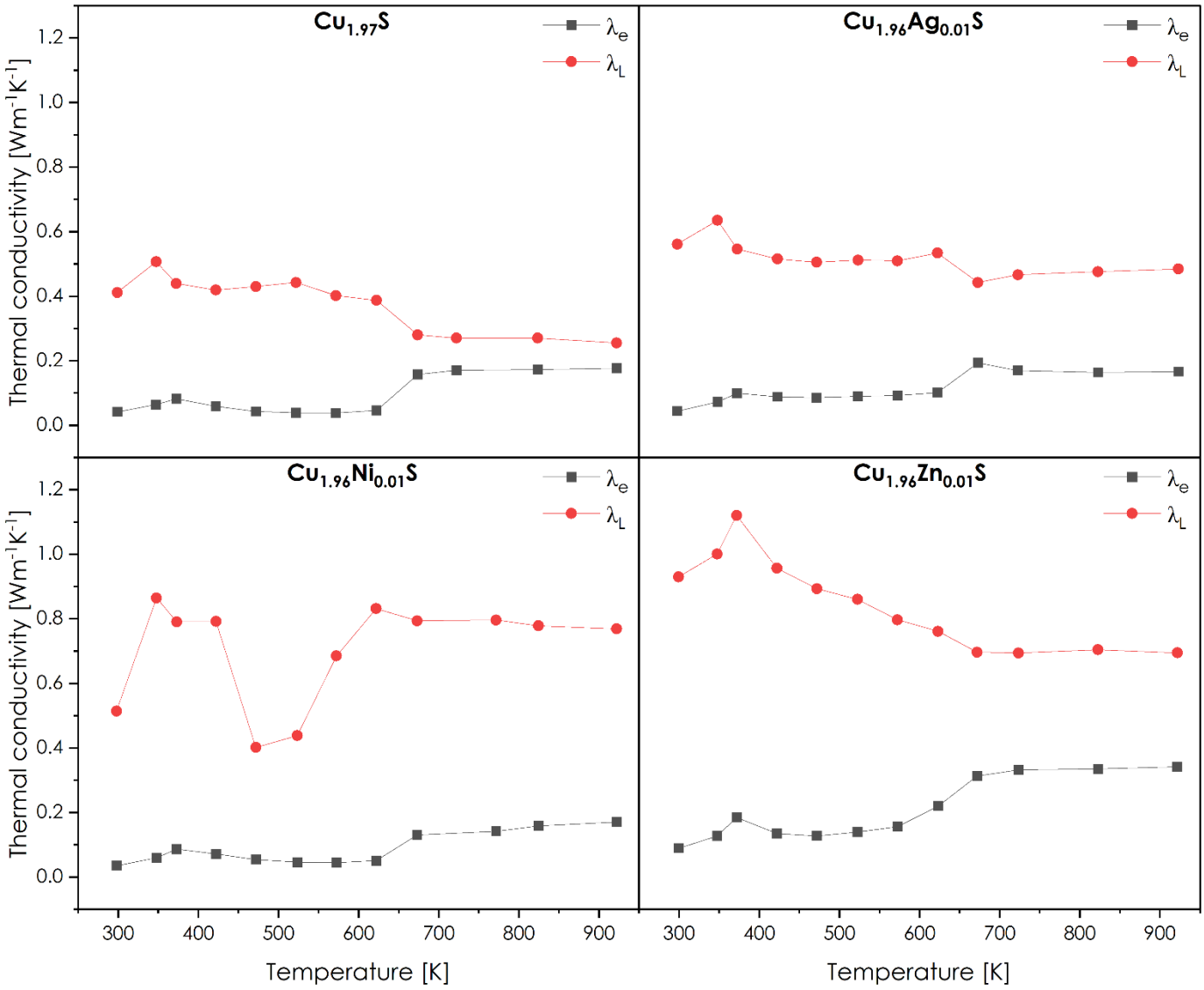


Figure S5. Lattice and electronic components of thermal conductivity as a function of temperature for copper (I) sulfides.

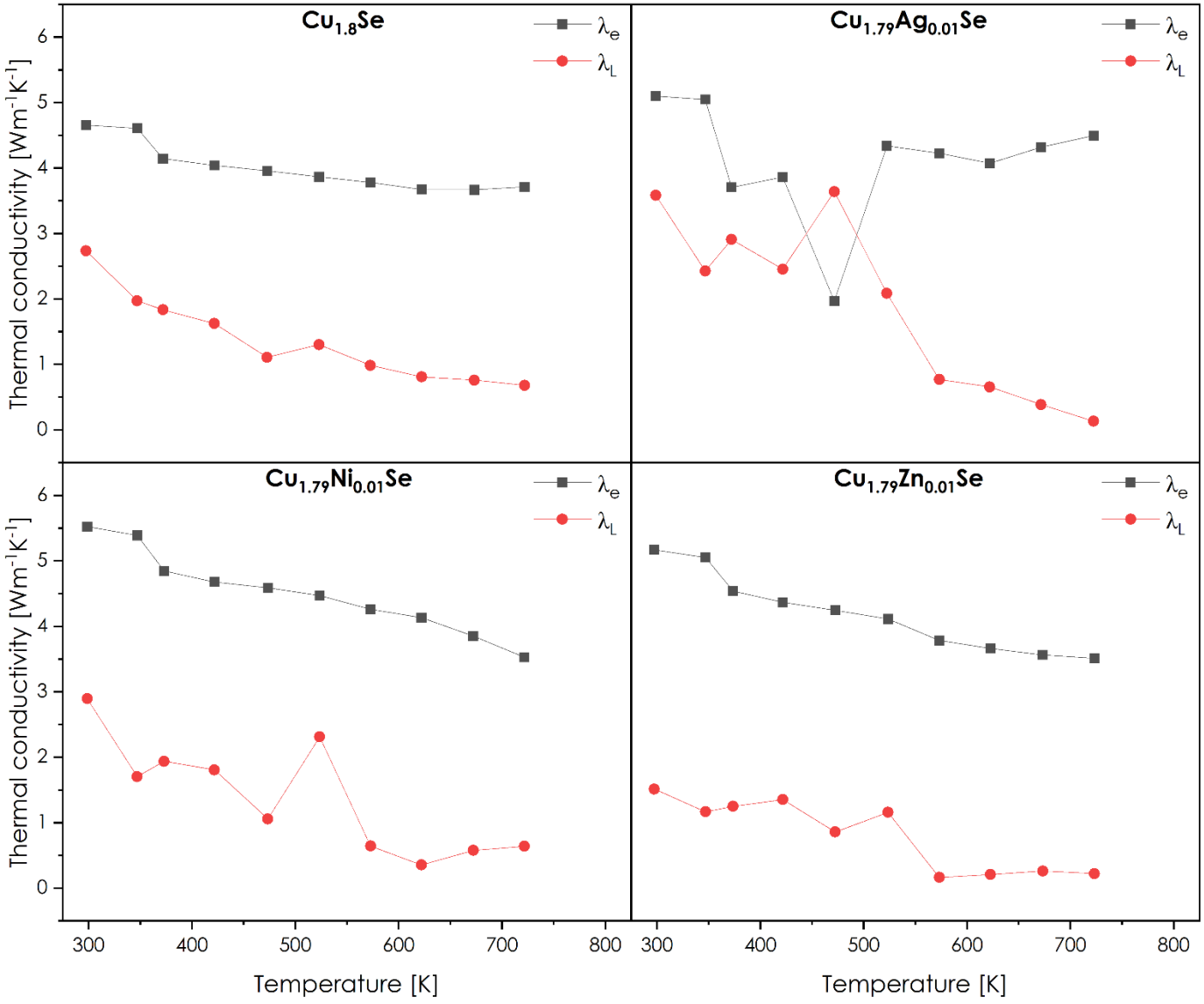


Figure S6. Lattice and electronic components of thermal conductivity as a function of temperature for copper (I) selenides.

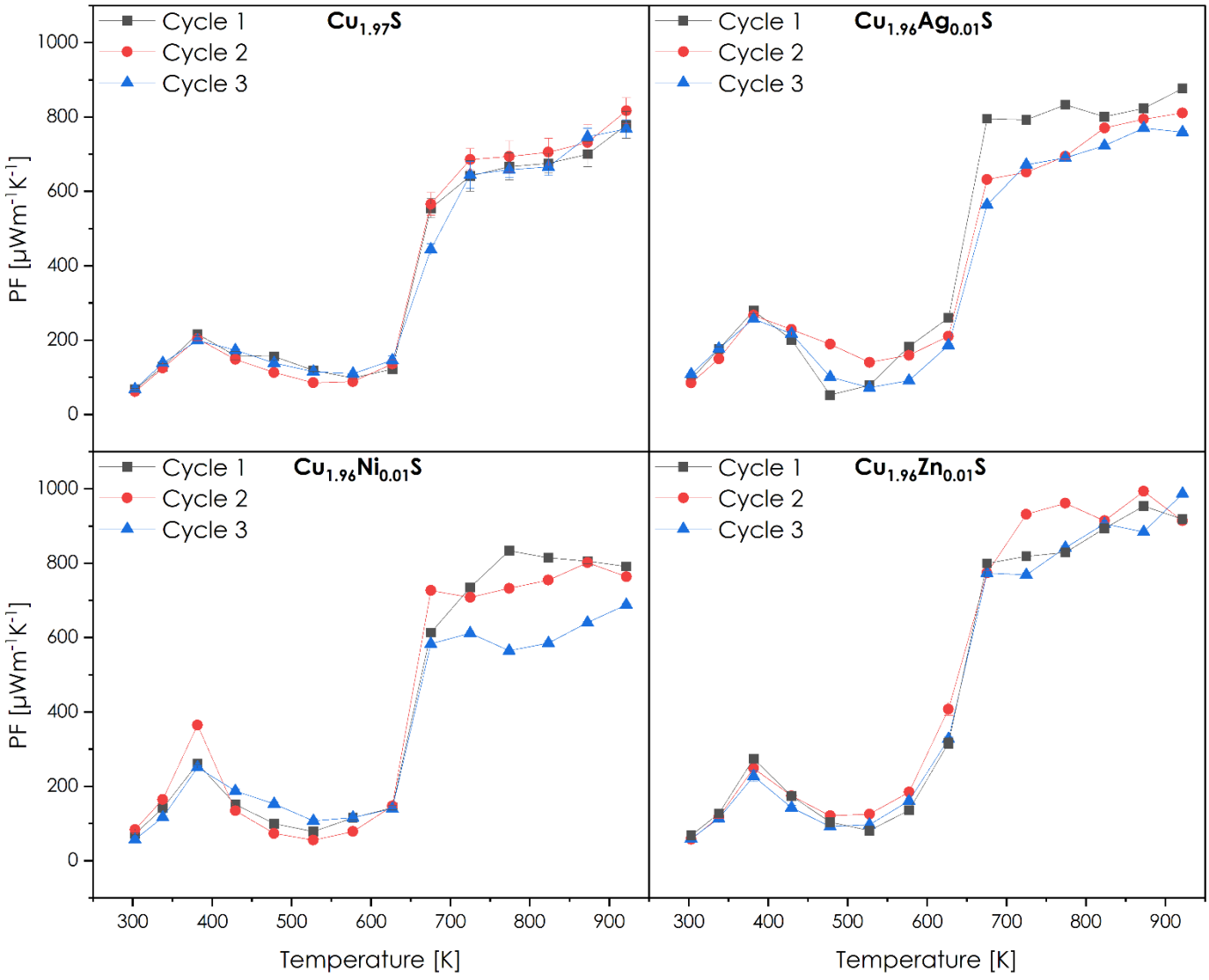


Figure S7. Power factor as a function of temperature for copper(I) sulfides.

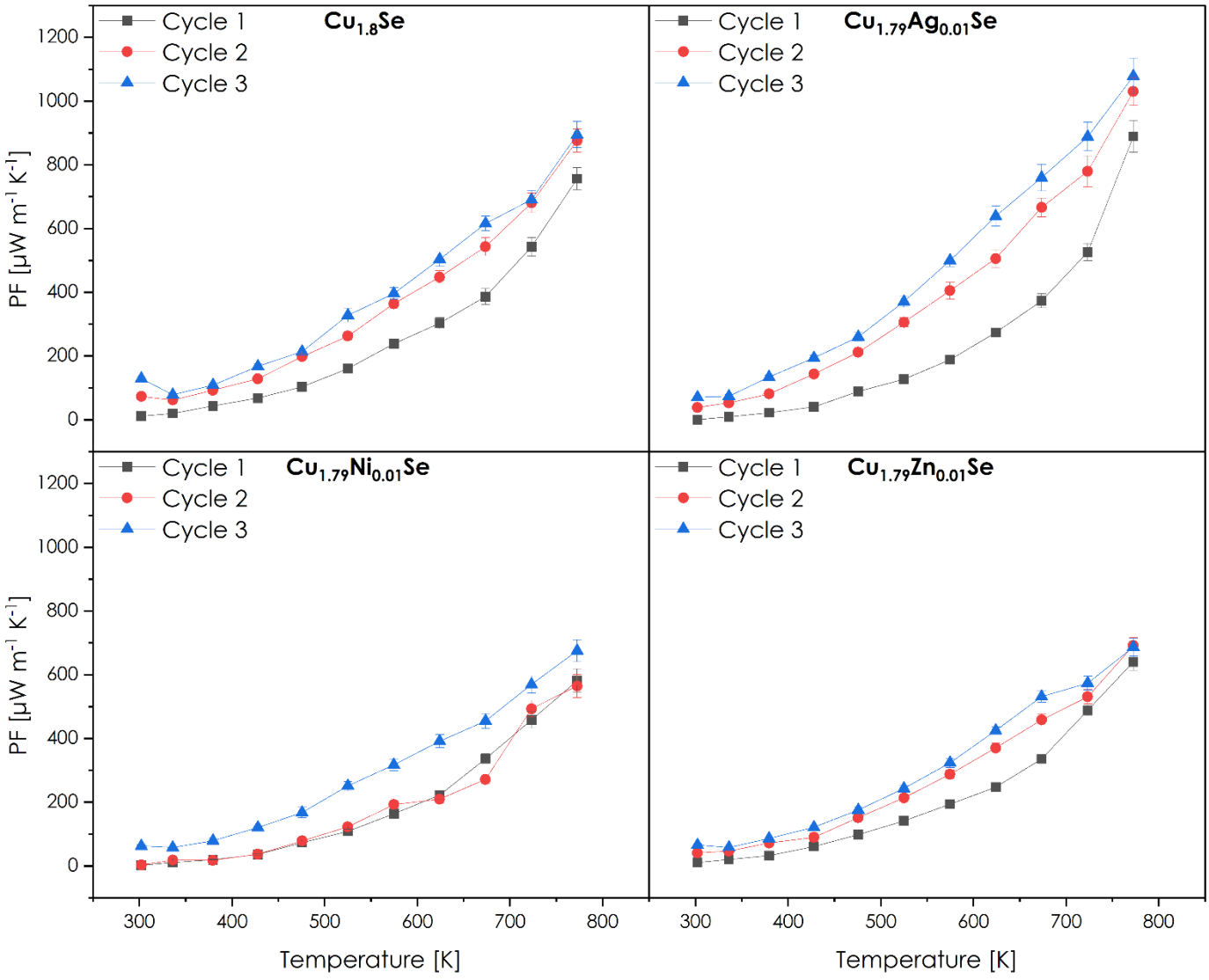


Figure S8. Power factor as a function of temperature for copper(I) selenides.

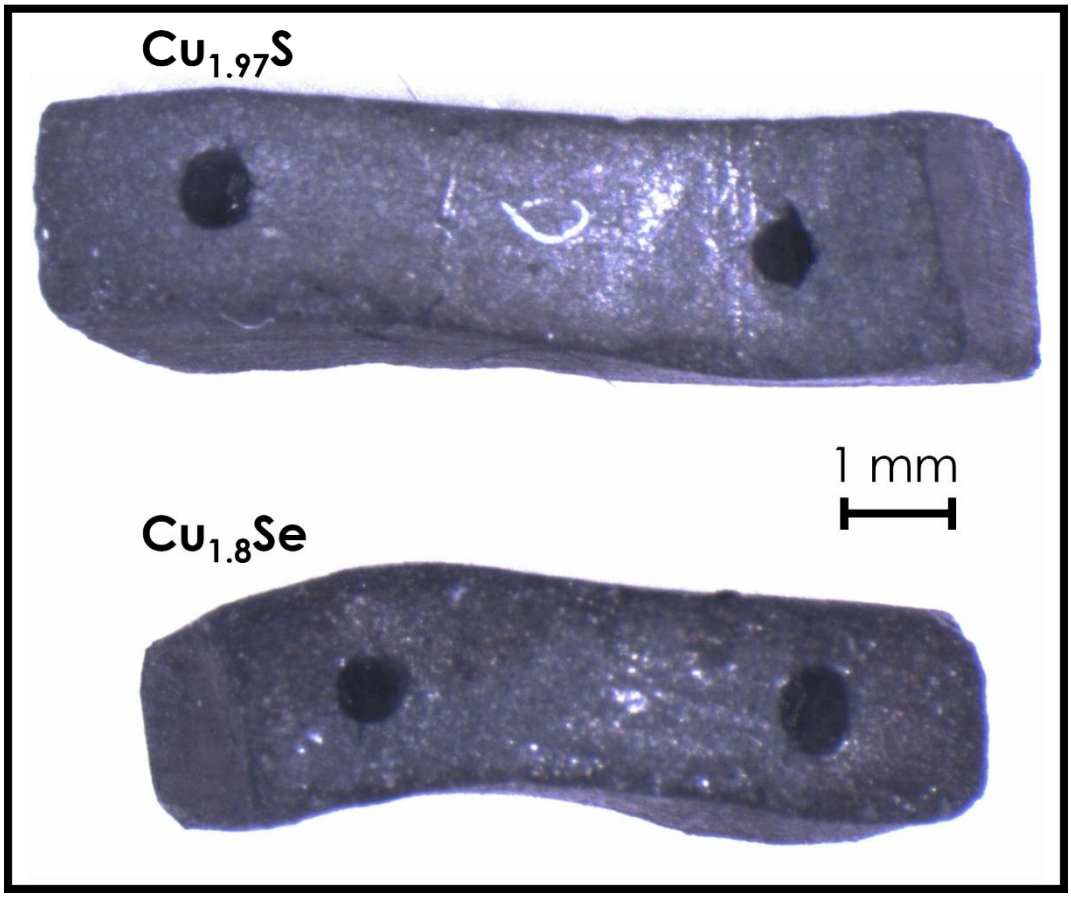


Figure S9. Optical microscope images of $Cu_{1.97}S$ and $Cu_{1.8}Se$ after TE measurements.