Ag doping induced abnormal lattice thermal conductivity in Cu$_2$Se

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1. Rietveld refinement calculated Cu$_2$O content and its influence on thermoelectric performance of Cu$_2$Se

Figure S1a and b show the experimental XRD patterns in comparison with the Rietveld refinement calculated ones of as-sintered (Cu$_{1-x}$Ag$_x$)$_2$Se pellets and the calculated Cu$_2$O ratios. The R$_{wp}$ values for (Cu$_{1-x}$Ag$_x$)$_2$Se with x=0, 0.005 and 0.01 are 7.9, 6.8 and 7.2 %, respectively. As can be seen, with increasing the Ag-doping level, the Cu$_2$O content increases up to 3.5 at. %. This fraction is lower than the critical point of ~7 at. %.\[1\] Below this point, Cu$_2$O has minor influence on thermoelectric performance of as-prepared (Cu$_{1-x}$Ag$_x$)$_2$Se.$[1]$

**Figure S1.** (a) Experimental and Rietveld refinement calculated XRD patterns and (b) Rietveld refinement calculated phase content of as-prepared Cu$_2$Se, (Cu$_{0.995}$Ag$_{0.005}$)$_2$Se and (Cu$_{0.99}$Ag$_{0.01}$)$_2$Se pellets.
2. Temperature-dependent specific heat of as-prepared (Cu_{1-x}Ag_{x})_2Se pellets

The temperature-dependent specific heat \((C_p)\) of as-prepared \((Cu_{1-x}Ag_{x})_2Se\) pellets are shown in Figure S2 (refer to Figure R2). The peaks at \(\sim 400\) K of all samples clearly revealed the well-known phase transition from \(\alpha-Cu_2Se\) to \(\beta-Cu_2Se\) at \(\sim 400\) K.[2, 3] Here, we are mainly focusing on thermoelectric performance of \((Cu_{1-x}Ag_{x})_2Se\) pellets after the phase transition where the temperature is higher than \(423\) K.

![Figure S2. Temperature \((T)\)-dependent specific heat \((C_p)\) of as-prepared \((Cu_{1-x}Ag_{x})_2Se\) pellets.](image-url)
Reference

