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Supporting Information

Giant enhancement of the figure-of-merit over a broad temperature range in nano-boron incorporated Cu_2Se

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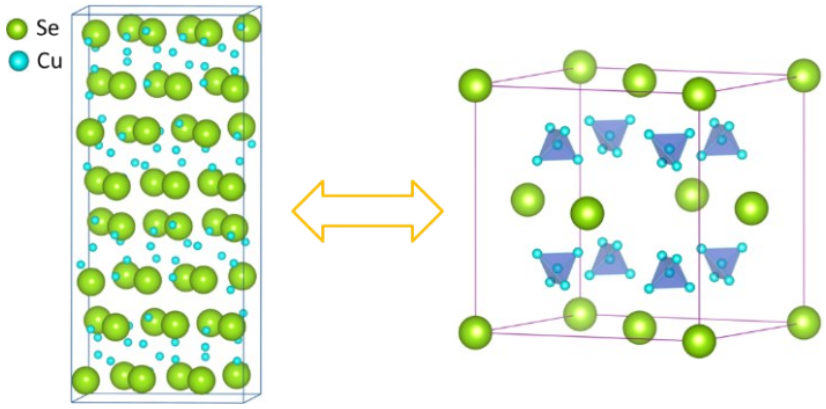

Fig. S1 Low-temperature monoclinic phase (left) and high-temperature cubic phase (right) of the Cu_2Se crystal structure

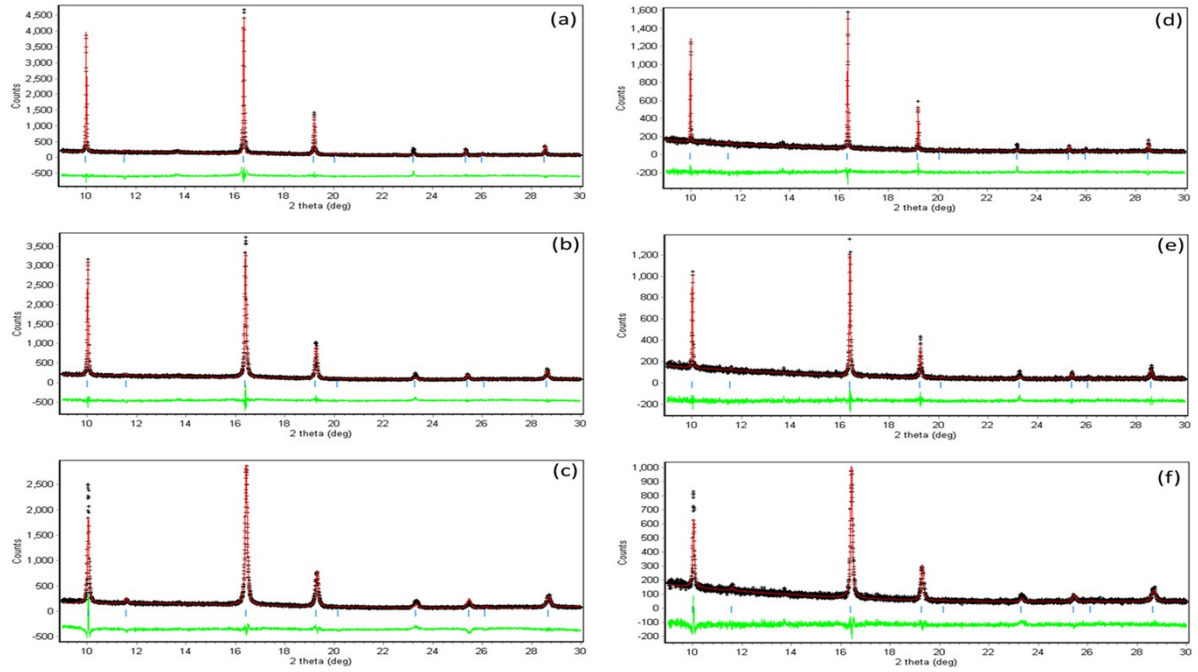

Fig. S2 Rietveld refinement of 0.42 wt% boron doped Cu_2Se (a-c) and undoped Cu_2Se (d-f) at 624 K, 512 K, and 403 K, respectively. The refined parameters are shown in Table S1.

Table S1 Parameters for the refinement of boron doped and undoped Cu_2Se at 624 K, 512 K, and 403 K. R_p and R_{wp} are the profile and weighted profile R-factors, respectively, and χ^2 is the goodness-of-fit.

Temp (K)	Lattice parameter / Sample	a (Å)	R_p	R_{wp}	χ^2
624	(a) 0.42 wt% Boron	5.85070	9.867	13.313	2.609
512	(b) 0.42 wt% Boron	5.83880	8.560	11.077	1.853
403	(c) 0.42wt% Boron	5.82770	9.858	12.999	2.579
624	(d) Cu_2Se	5.86110	9.777	12.962	1.242
512	(e) Cu_2Se	5.84270	9.325	12.175	1.157
403	(f) Cu_2Se	5.83160	9.517	12.165	1.283

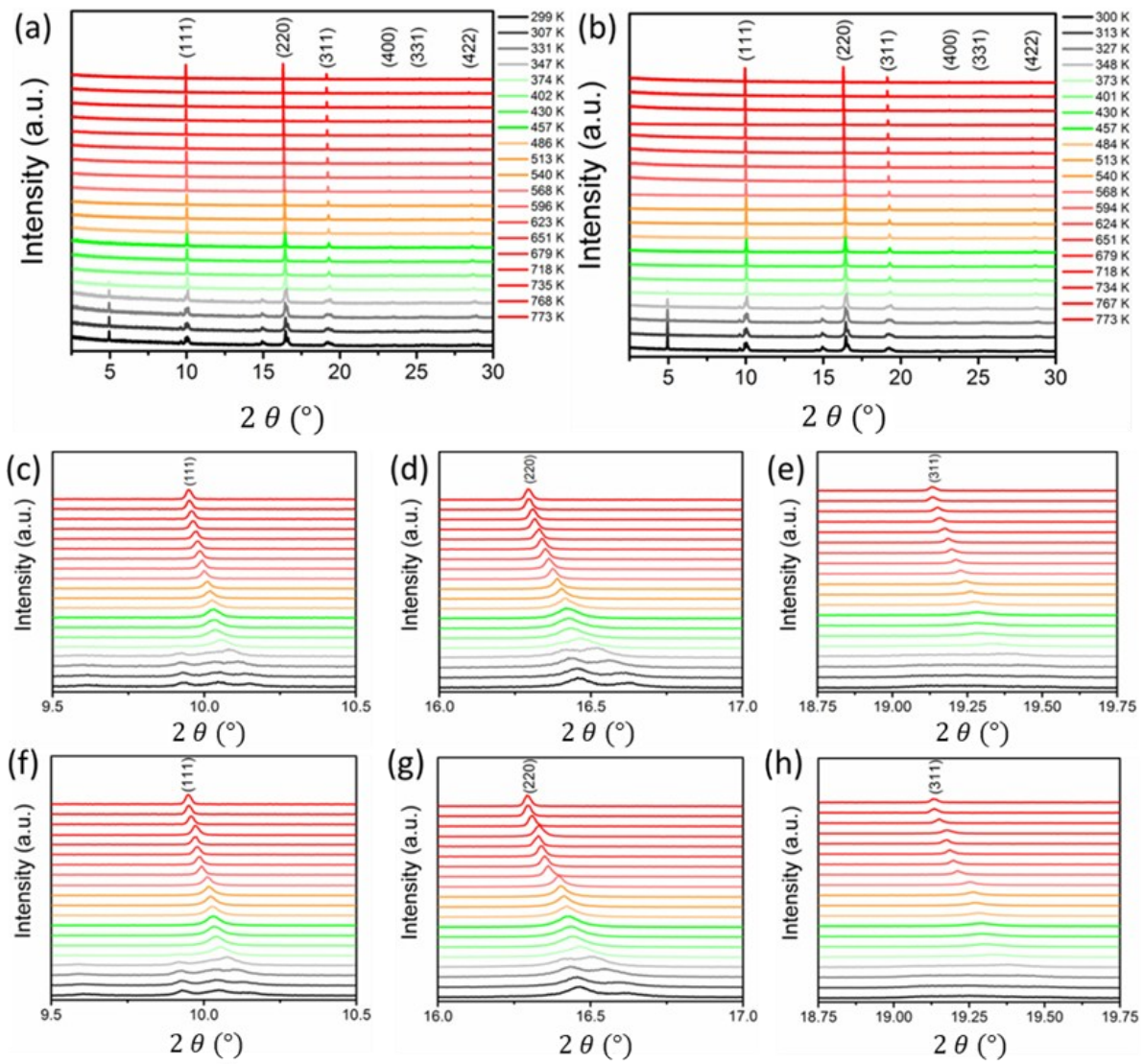

Fig. S3 Synchrotron powder diffraction patterns over the entire measured temperature range of ~300–773 K for 2θ = a) 2.5°–30° (Undoped), b) 2.5°–30° (0.42 wt% Boron) c) 9.5°–10.5° (Undoped), d) 16°–17° (Undoped), e) 18.75°–19.75° (Undoped), f) 9.5°–10.5° (Boron), g) 16°–17° (Boron), h) 18.75°–19.75° (Boron). The wavelength is 0.5897313 Å.

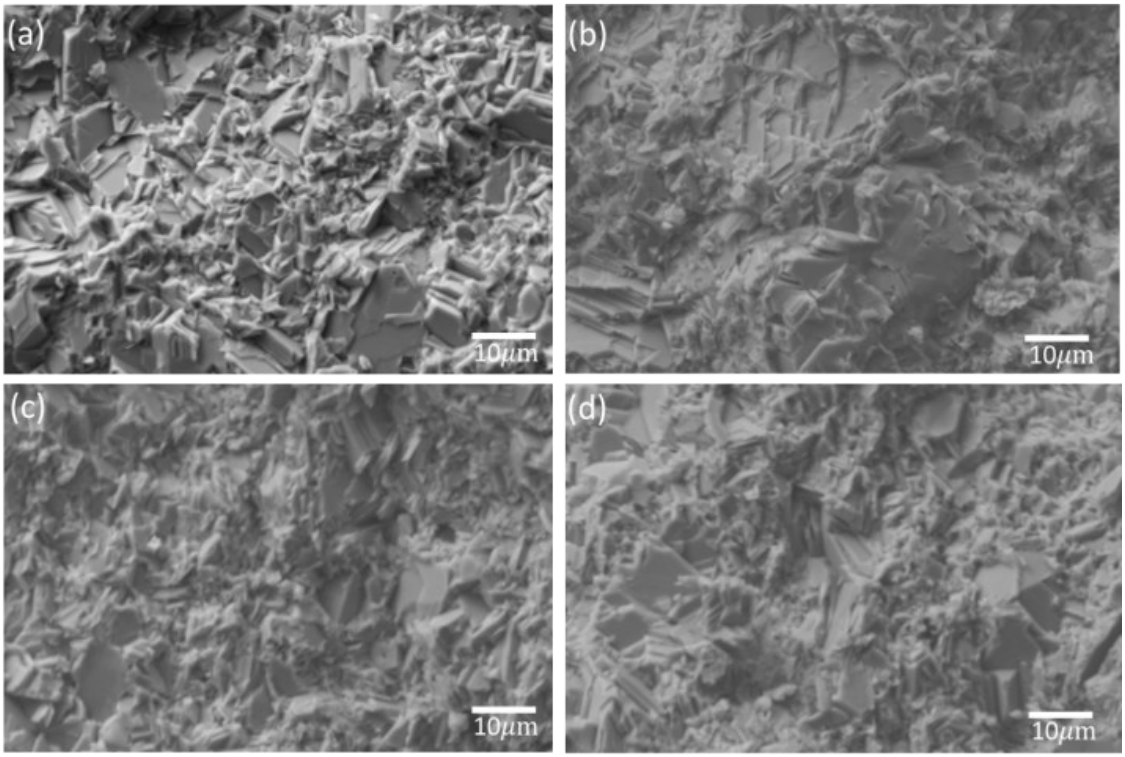

Fig. S4 SEM images of fractured surface morphology of (a) pure Cu_2Se, and b) 0.14 wt%, (c) 0.28 wt%m and (d) 0.42 wt% boron-doped polycrystalline Cu_2Se fabricated by the spark plasma sintering (SPS) method.

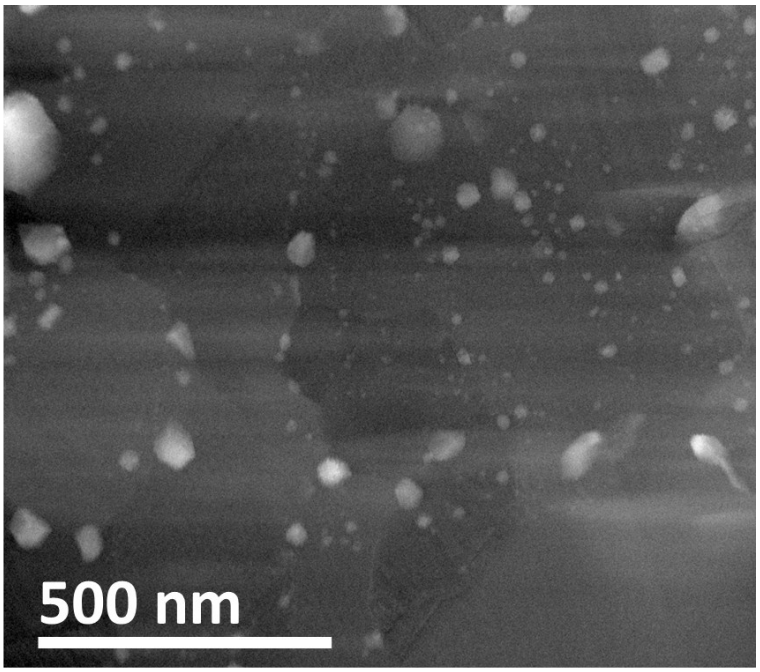

Fig. S5 Low magnification TEM image of the boron doped Cu_2Se bulk sample showing the presence of boron across the grain boundary

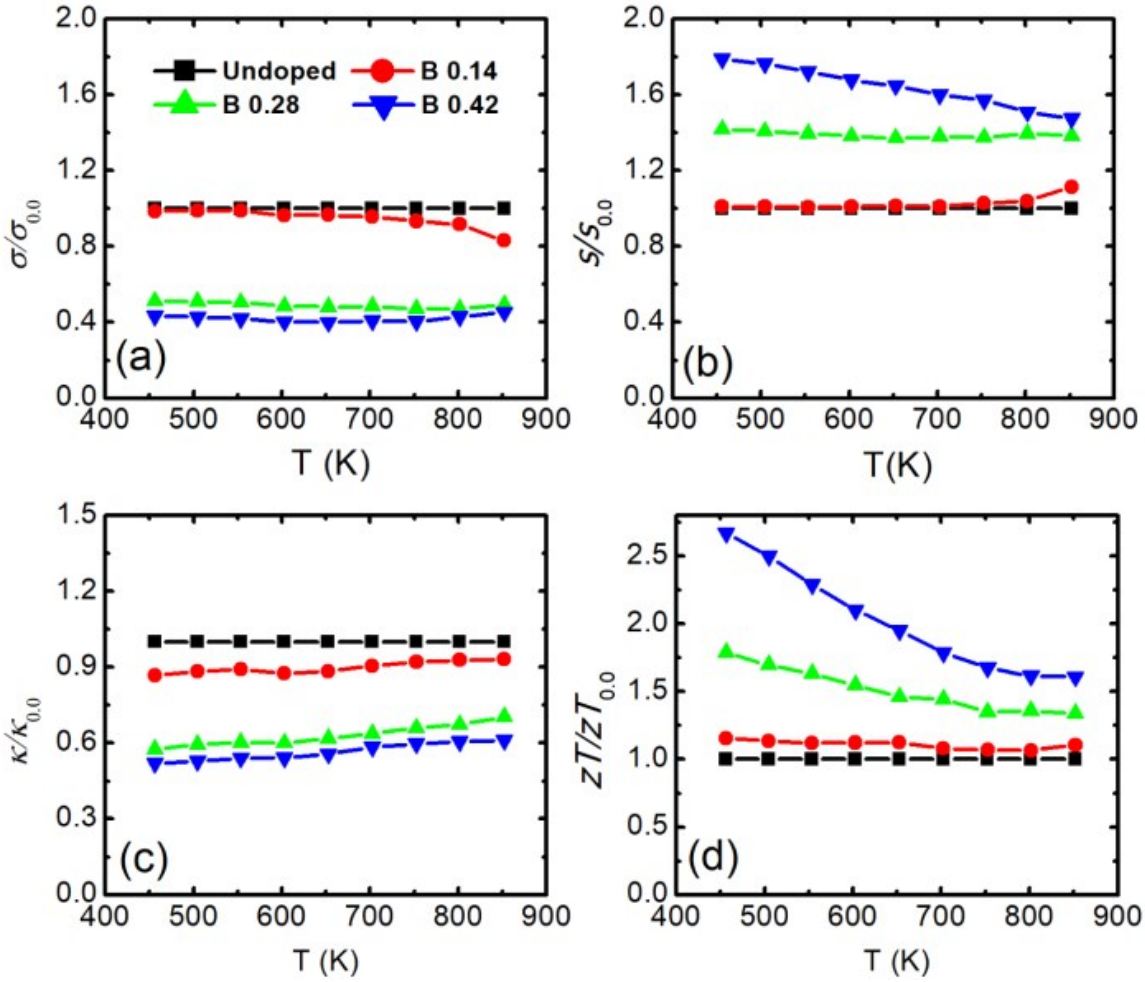

Fig. S6 Temperature dependence of (a) $\sigma/^{\sigma}_{0.0}$, (b) $S/S_{0.0}$, (c) $\kappa/\kappa_{0.0}$, and (d) $zT/zT_{0.0}$ for the boron doped Cu_2Se samples with doping levels of 0.14, 028, and 0.42 wt%.

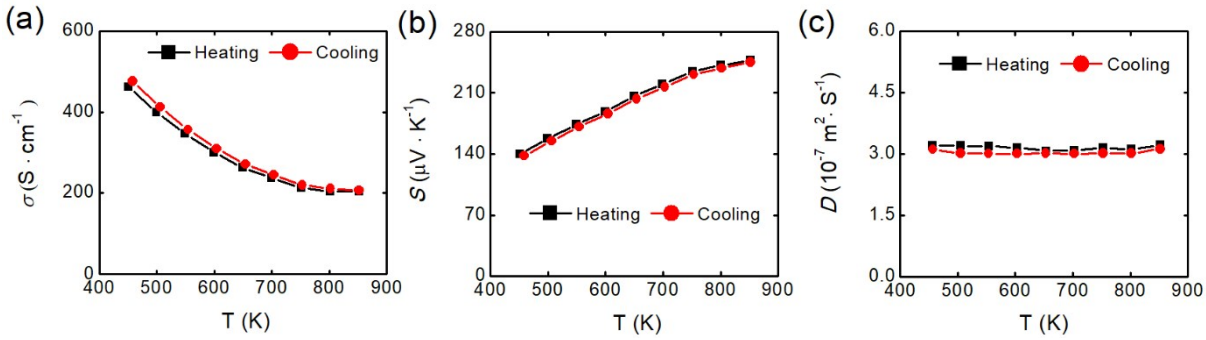

Fig. S7 The electrical and thermal transport properties with respect to temperature during heating up and cooling down for a 0.42 wt.% Boron doped Cu_2Se sample: (a) electrical conductivity (σ); (b) Seebeck coefficient (S); (c) thermal diffusivity (D).