

Supporting Information

Synergistic Enhancement of Cu₂Se Thermoelectric Properties via *Te* and *S* Co-doping: Aqueous Synthesis and Cold-Press Sintering for Power Generation

Vinothkumar Lourdhusamy¹, Immanuel Paulraj¹, Veera Prabu Kannan², and Chia-Jyi Liu^{1,*}

¹Department of Physics, National Changhua University of Education, Changhua 500, Taiwan

²Department of Metallurgical and Materials Engineering, IIT Madras, Chennai 600036,
Tamil Nadu, India

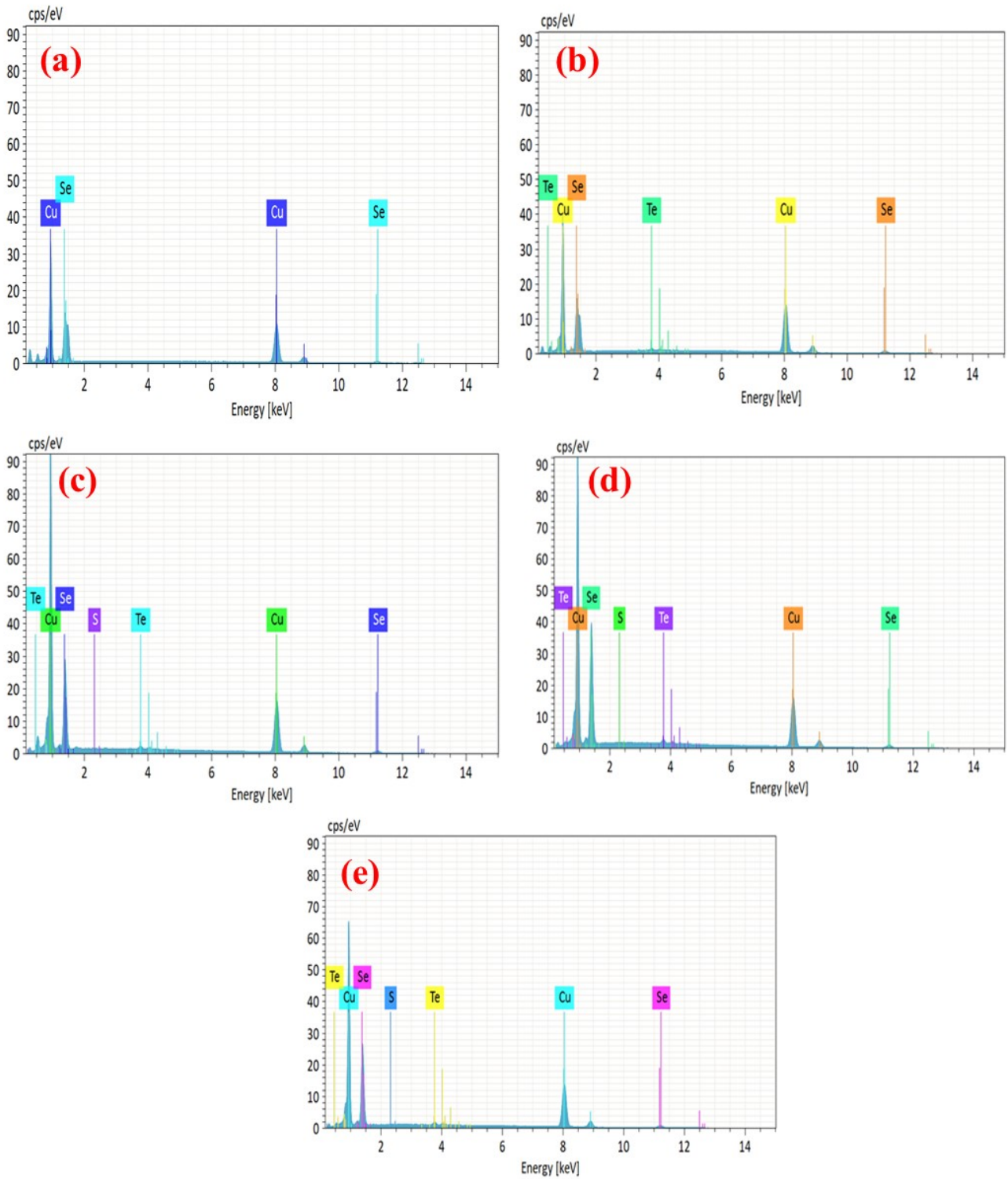


Fig. S1 EDAX of (a) Cu_2Se , (b) $\text{Cu}_2\text{Se}_{0.96}\text{Te}_{0.04}$, (c) $\text{Cu}_2\text{Se}_{0.95}\text{S}_{0.01}\text{Te}_{0.04}$, (d) $\text{Cu}_2\text{Se}_{0.94}\text{S}_{0.02}\text{Te}_{0.04}$, (e) $\text{Cu}_2\text{Se}_{0.93}\text{S}_{0.03}\text{Te}_{0.04}$.

The weighted mobility of the Cu_2Se and $\text{Cu}_2\text{Se}_{0.96-x}\text{S}_x\text{Te}_{0.04}$ (where $x = 0.00, 0.01, 0.02,$ and 0.03) was determined using

$$\mu_w = \frac{3 h^3}{8 \pi e \rho (2 m_e k_B T)^{3/2}} \left[\frac{\text{Exp} \left[\frac{|S|}{k_B} - 2 \right]}{1 + \text{Exp} \left[-5 \left(\frac{|S|}{k_B} - 1 \right) \right]} + \frac{\frac{3 |S|}{\pi^2 k_B}}{e} \right] \frac{1}{1 + \text{Exp} \left[5 \left(\frac{|S|}{k_B} - 1 \right) \right]}, \quad (\text{S1})$$

where h , e , ρ , k_B , m_e , S , and T are Plank's Constant, the carrier's charge, electrical resistivity in $\text{m}\Omega\text{-cm}$, the Boltzmann constant, the electron's rest mass, Seebeck coefficient, and absolute temperature, respectively.

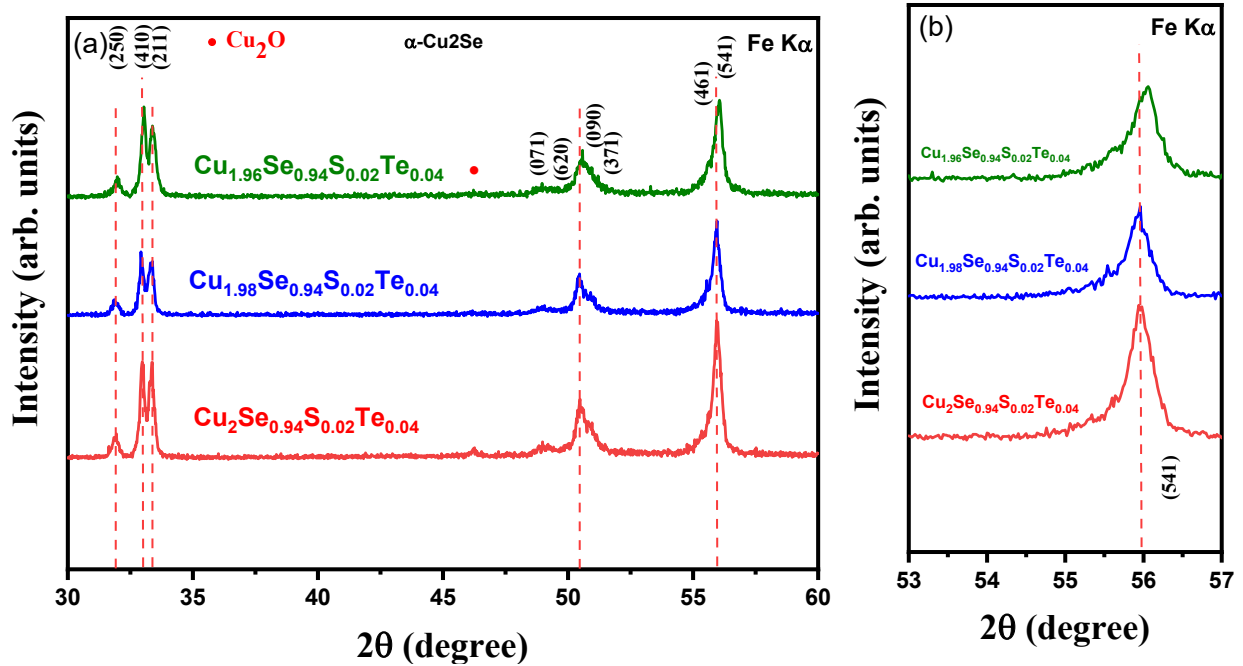


Fig. S2 XRD patterns of $\text{Cu}_{2-y}\text{Se}_{0.94}\text{S}_{0.02}\text{Te}_{0.04}$ ($y = 0.00, 0.02,$ and 0.04) (a) sintered at 923 K for 6 h in vacuum; (b) with an expanded view for greater detail.

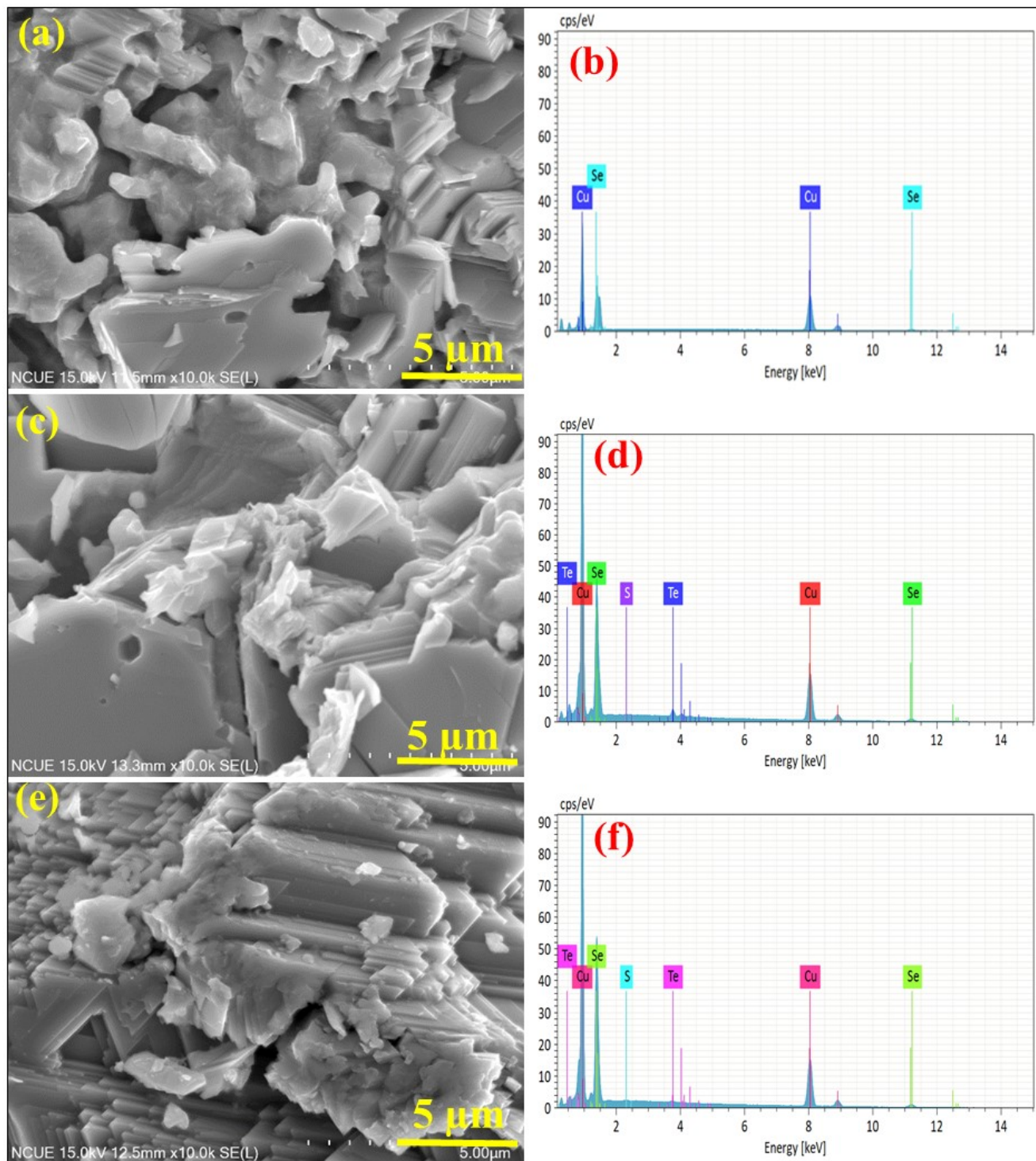


Fig. S3 FE-SEM and EDAX analysis of (a-b) $\text{Cu}_2\text{Se}_{0.94}\text{S}_{0.02}\text{Te}_{0.04}$; (c-d), $\text{Cu}_{1.98}\text{Se}_{0.94}\text{S}_{0.02}\text{Te}_{0.04}$; (e-h) $\text{Cu}_{1.96}\text{Se}_{0.94}\text{S}_{0.02}\text{Te}_{0.04}$ of sintered at 923 K for 6 h in vacuum.

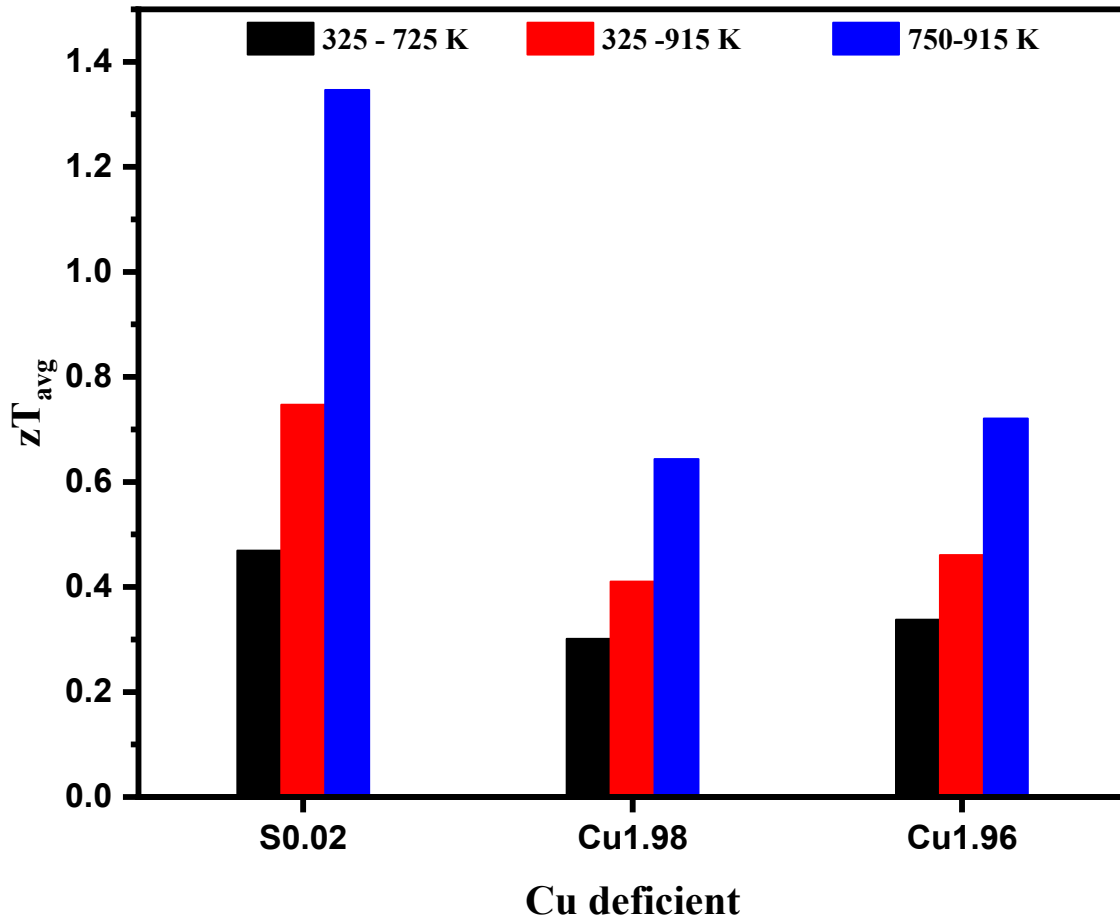


Fig. S4 Average zT (zT_{avg}) for $\text{Cu}_{2-y}\text{Se}_{0.94}\text{S}_{0.02}\text{Te}_{0.04}$ with $y = 0.00, 0.02, \text{ and } 0.04$ sintered at 923 K for 6 h in vacuum.

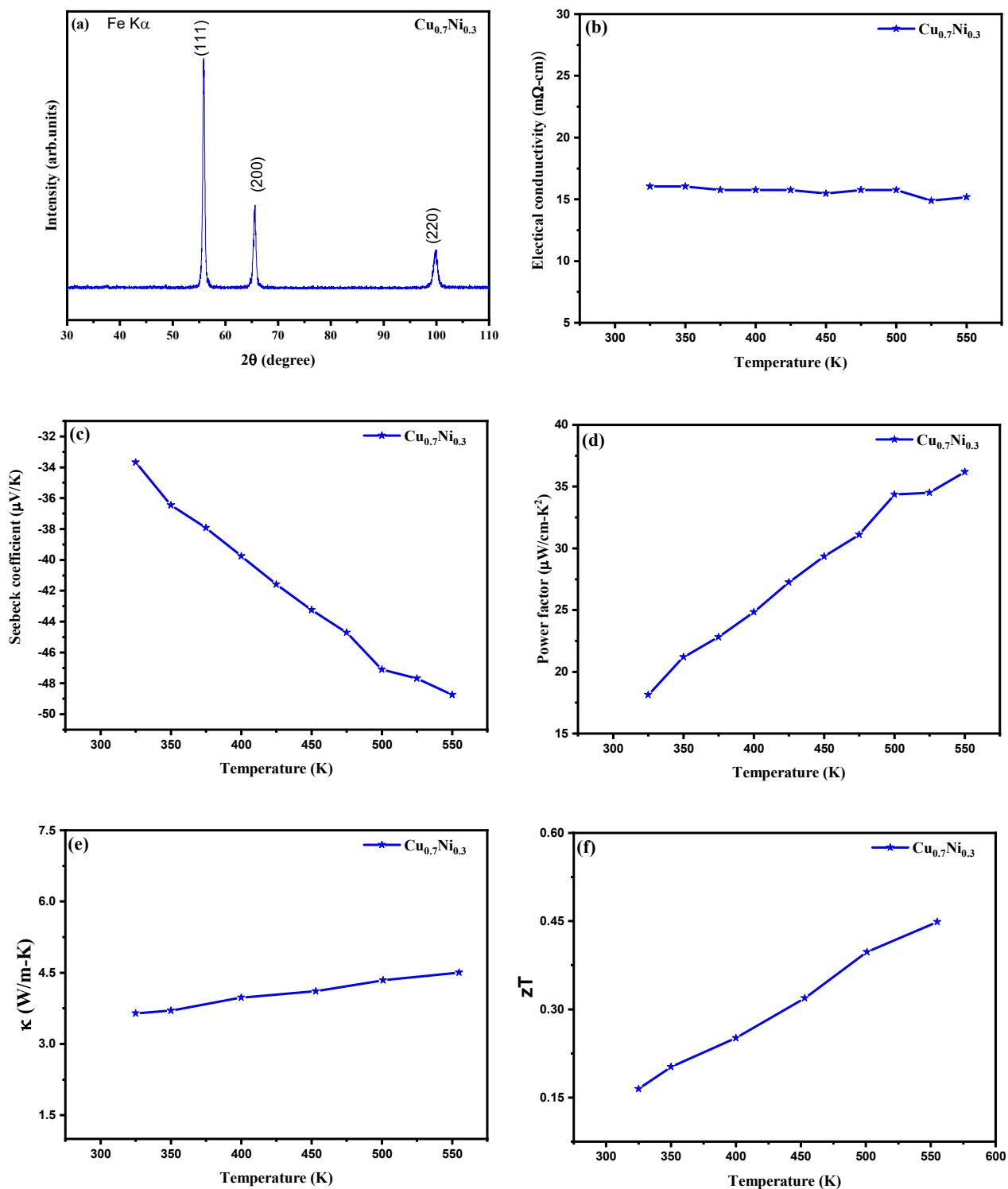


Fig. S5 The $\text{Cu}_{0.7}\text{Ni}_{0.3}$. (a) X-ray diffraction pattern (b) electrical conductivity; (c) Seebeck coefficient; (d) power factor; (e) total thermal conductivity; (f) zT .

