Electronic Supplementary Information (ESI)

Effect of Order-Disorder Phase Transition and Band Gap Evolution on the Thermoelectric Properties of AgCuS Nanocrystals†

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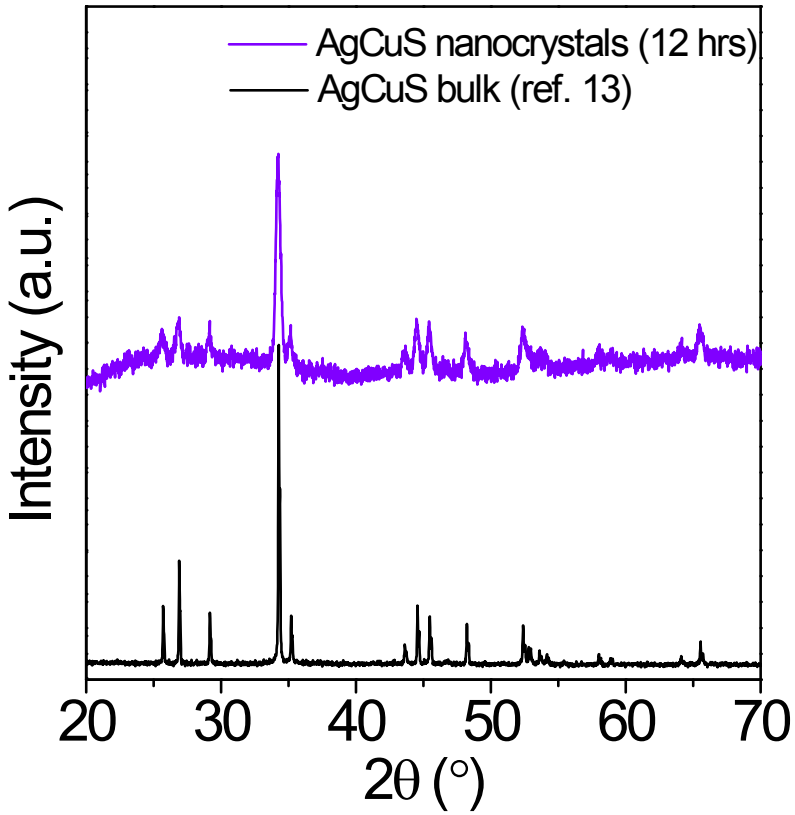

Fig. S1 Powder XRD pattern for AgCuS nanocrystals obtained after 12 hrs of reaction time measured at lab source (Cu K_α; λ = 1.5406 Å) with PXRD of bulk AgCuS.[13]

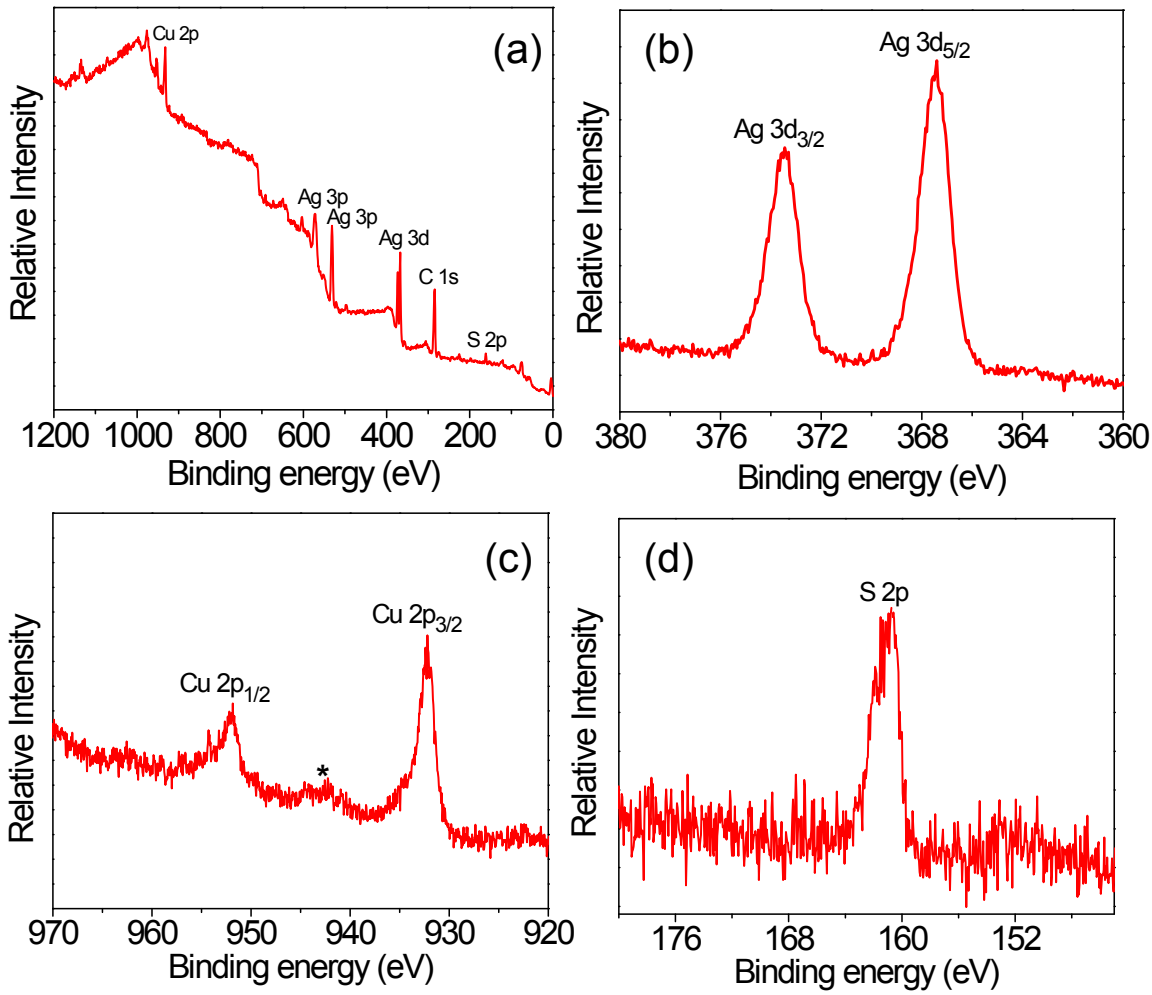

Fig. S2 XPS spectra of AgCuS nanocrystals (30 min reaction) (a) XPS survey scan (b) Ag 3d, (c) Cu 2p and (d) S 2p spectra. An additional peak (* marked) in Cu 2p was due to presence of small amount of Cu(II).

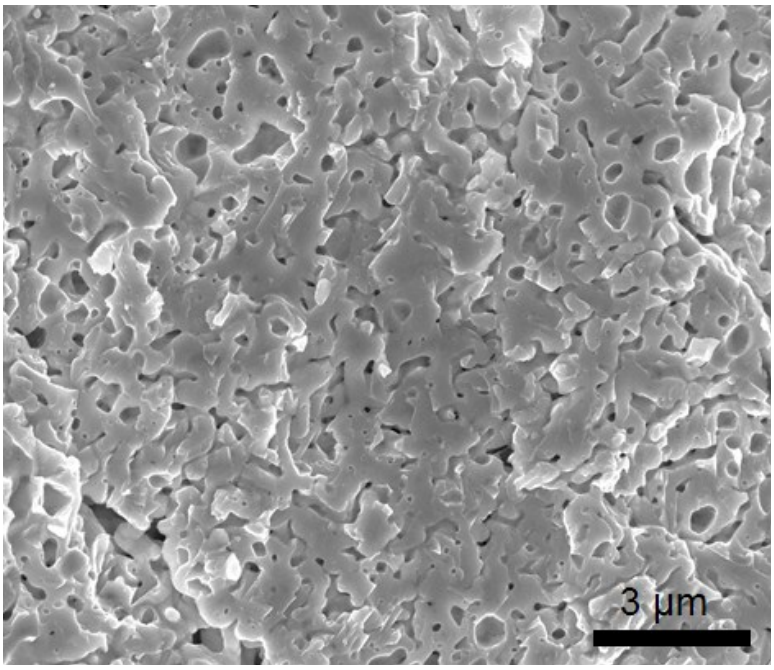

Fig. S3 FESEM image after sintering of AgCuS nanocrystals at 573 K for 3 hrs.

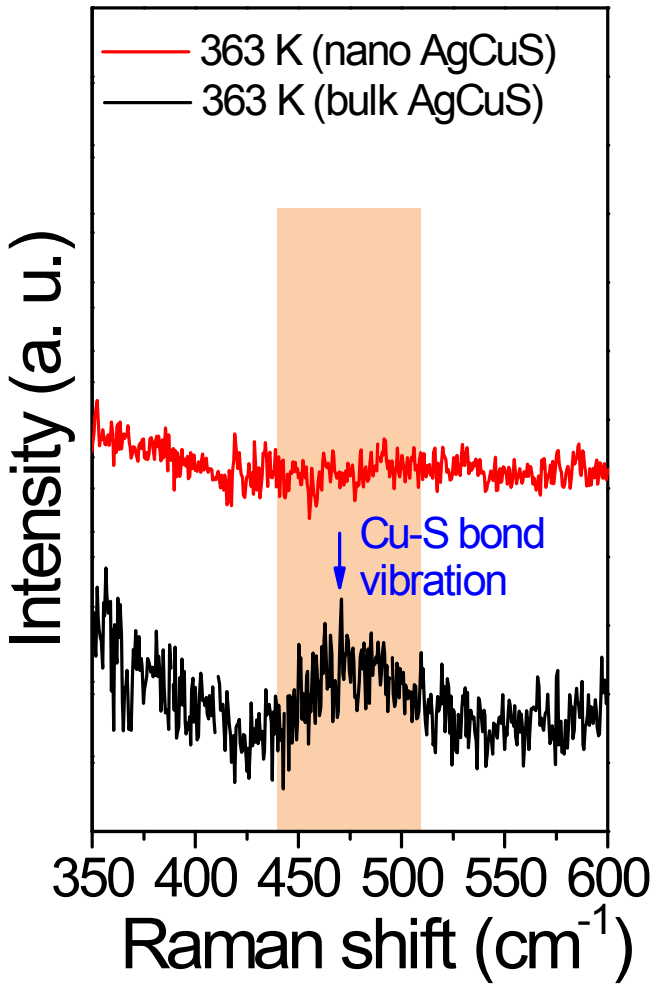

Fig. S4 Raman spectra of bulk and nanocrystalline AgCuS (30 min reaction), in the range of 350-600 cm^{-1}, indicating the absence of Cu-S bond vibration in nanocrystalline sample during orthorhombic (β) to hexagonal phase (α) transition.

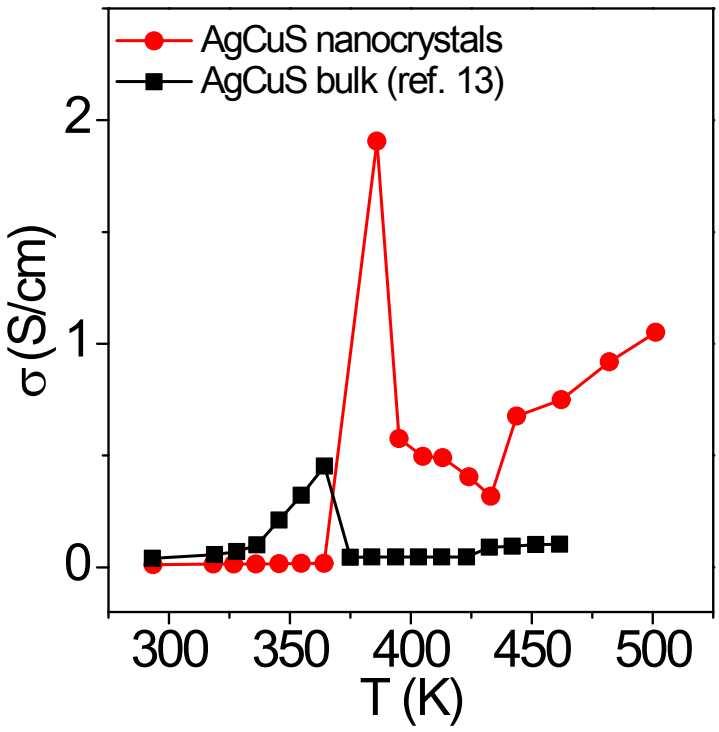

Fig. S5 Temperature dependent electrical conductivity (σ) of nanocrystalline AgCuS compared with its bulk counterpart[13].

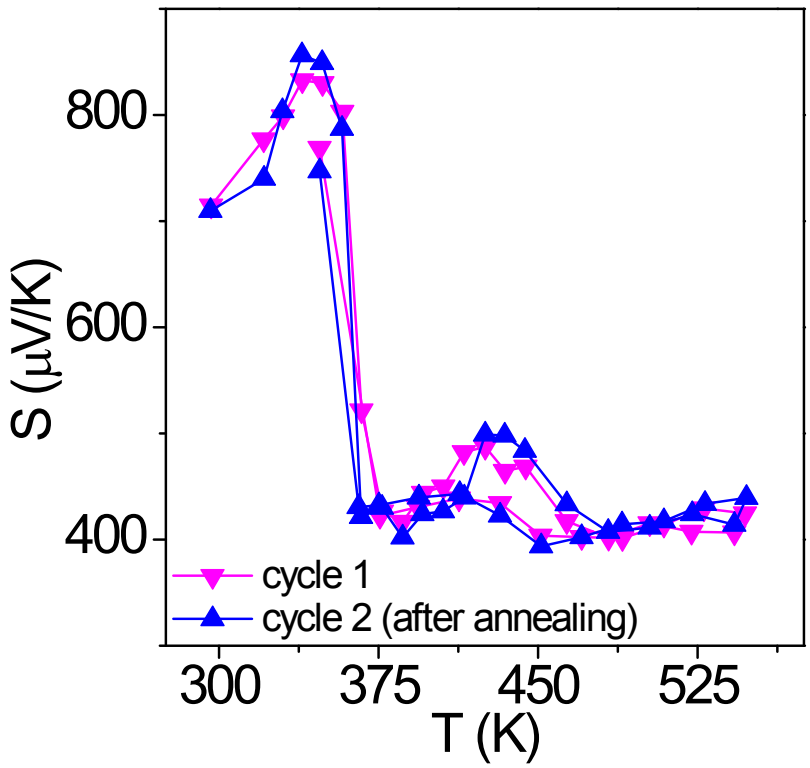

Fig. S6 Temperature dependent two cycle heating cooling Seebeck coefficient data for nanocrystalline AgCuS (30 min reaction).

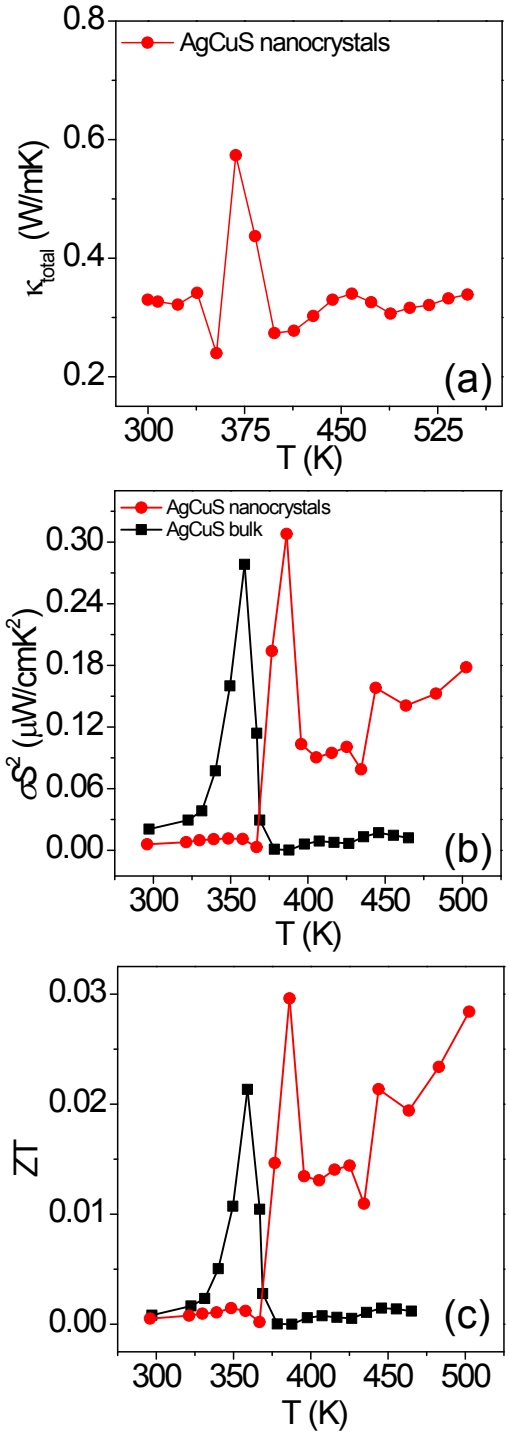

Fig. S7 Temperature dependent (a) thermal conductivity (κ_{total}) of AgCuS nanocrystals obtained after 30 min of reaction. (b) and (c) are comparative temperature dependent power factor (σS^2) and thermoelectric figure of merit (*ZT*) of bulk and nanocrystalline AgCuS, respectively.

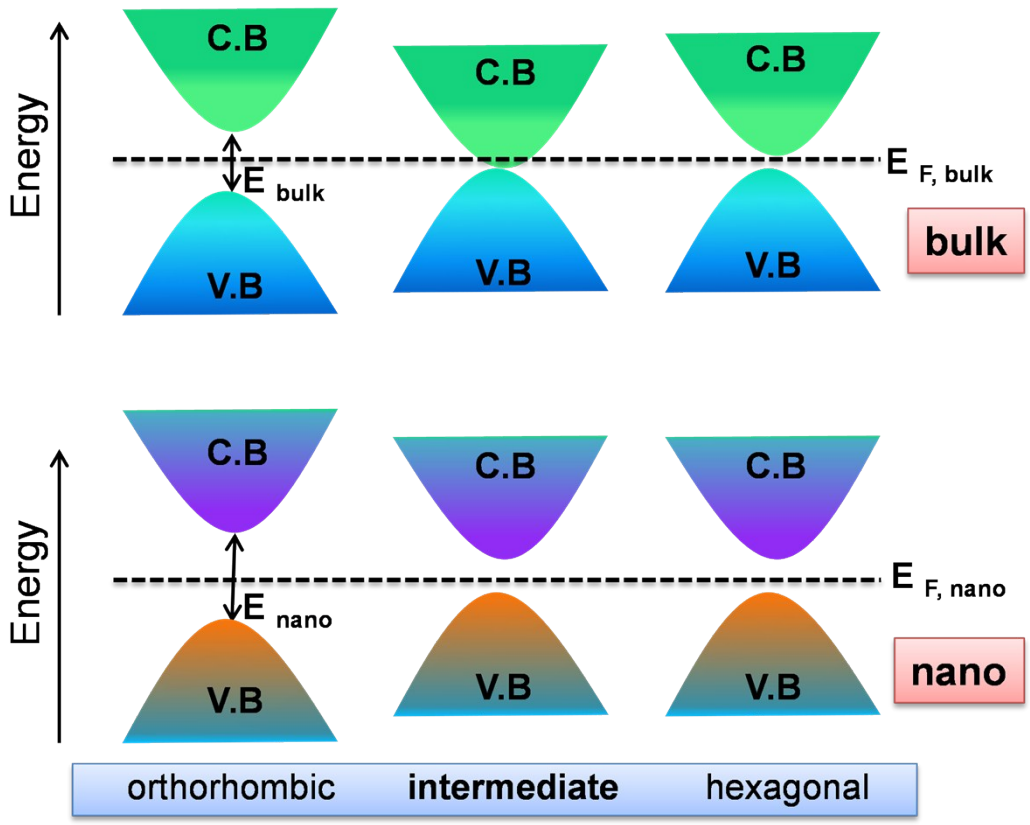

Fig. S8 Schematic representation of changes of the band gap of bulk and nanocrystalline AgCuS during orthorhombic (β) to hexagonal (α) phase transition.