

Supporting Information

Nanostructured monoclinic Cu₂Se as near-room-temperature thermoelectric materials

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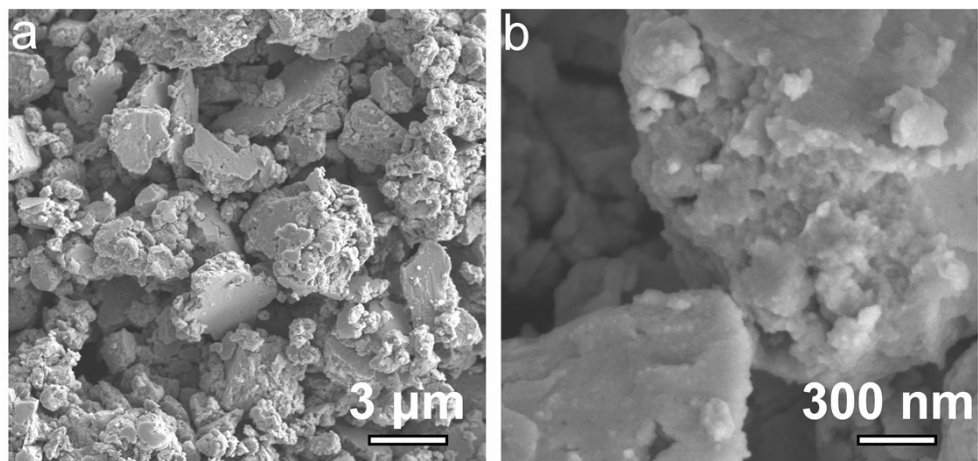


Figure S1. SEM images of the as-prepared nano β - Cu_2Se powders.

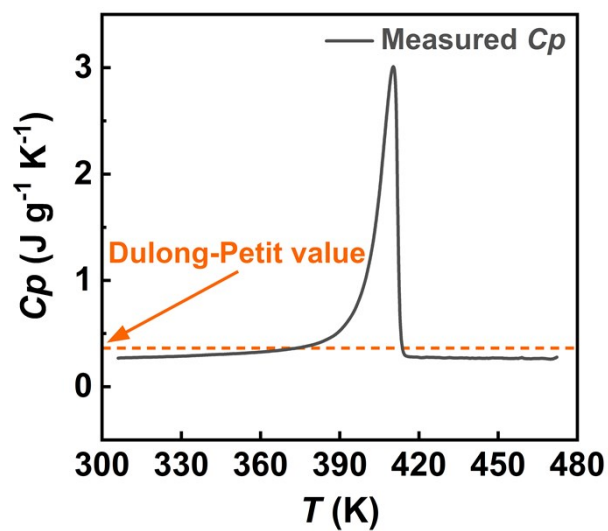


Figure S2. The measured C_p as a function of T compared with the Dulong-Petit value, which shows that the Dulong-Petit value can well describe the C_p of our sample before phase transition temperature.

Calculation details of Debye-Callaway model:

The relevant phonon relaxation times are given by:

Umklapp processes

$$\tau_U^{-1} = AT \exp(-\theta_D / 3T) \omega^2 \quad \backslash * \text{MERGEFORMAT (1)}$$

Grain boundary scattering

$$\tau_B^{-1} = \frac{v}{L} \quad \backslash * \text{MERGEFORMAT (2)}$$

Point defect scattering

$$\tau_{PD}^{-1} = \frac{\bar{V} \Gamma}{4\pi v^3} \omega^4 \quad \backslash * \text{MERGEFORMAT (3)}$$

Phonon resonance scattering

$$\tau_{PR}^{-1} = \sum_i \frac{C_i \omega^2}{(\omega_i^2 - \omega^2)^2} \quad \backslash * \text{MERGEFORMAT (4)}$$

In the above equations, A is the fitted parameter in Umklapp processes, L is the grain size, $\bar{V} = 10^{-6} M / (D_T N_A n)$ is the average atomic volume (where M is the relative molecular mass, D_T is the theoretical density, N_A is the Avogadro constant, n is the number of atoms in a molecular formula), Γ is the point defect scattering parameter (fitted), C_i is the fitted parameters in phonon resonance scattering, ω_i is the resonant phonon frequency.

In this work for our nano Cu_2Se , $A = 6.5 \times 10^{-17} \text{ s K}^{-1}$ (fitted), $L = 45 \text{ nm}$, $M = 206.052 \text{ g mol}^{-1}$, $D_T = 6.749 \text{ g cm}^{-3}$, $n = 3$, $\Gamma = 0.3765$ (fitted), v , θ_D , and parameters in

phonon resonance scattering are taken from the reference.¹

Reference

1. H. L. Liu, J. Yang, X. Shi, S. A. Danilkin, D. H. Yu, C. Wang, W. Q. Zhang and L. D. Chen, *J. Materiomics*, 2016, **2**, 187-195.