

Thermal conductivity of PbTe-CoSb₃ bulk polycrystalline composite: the role of
microstructure and interface thermal resistance

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Table S1. Milling parameters for preparation of PbTe and CoSb₃ powders

~300 μm (CoSb ₃)	Hand grinding in a mortar, sieving (<300 μm , >100 μm) and decantation of the solution in isopropanol to separate the desired fraction from residual small grains		
~30 μm (CoSb ₃ and PbTe)	Ball milling (agate jar and balls $\phi=10\text{mm}$)	500 rpm	15 minutes
~1 μm (CoSb ₃)	Ball milling (agate jar and balls $\phi=3\text{mm}$)		6 hours

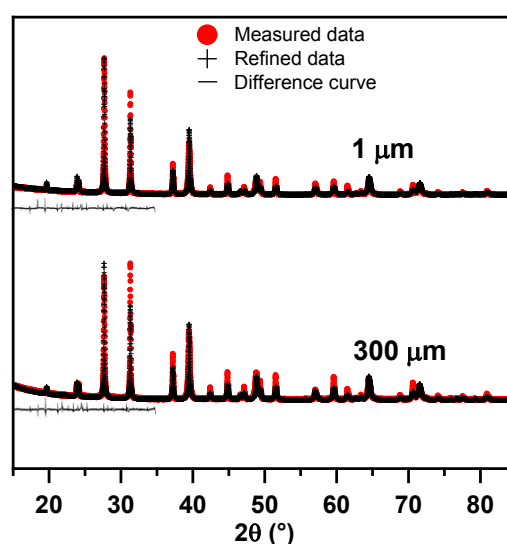


Figure S1. XRD patterns and Rietveld refinement results for the (0.5)PbTe/(0.5)CoSb₃ composite for different grain sizes of CoSb₃ phase

Lorenz number calculation

Table S2. Material parameters used for calculation of the Lorenz number.

	PbTe [1][2]	CoSb₃ [3]
Effective mass	0.24m _e	4m _e
Band gap [eV]	0.31	0.06

Nonparabolicity of the bands in PbTe and CoSb₃ has an impact on the electronic contribution to lattice thermal conductivity [4,5]. Thus, the Kane band model [1][6] was used for calculation of the Lorenz number with the following equations:

$$L_0(\eta, \beta) = \left(\frac{k_B}{e}\right)^2 \left[\frac{I_{r+1,2}^2(\eta, \beta)}{I_{r+1,2}^0(\eta, \beta)} - \left(\frac{I_{r+1,2}^1(\eta, \beta)}{I_{r+1,2}^0(\eta, \beta)} \right)^2 \right], \quad (1)$$

where k_B and e denote Boltzmann constant and elementary charge, $I_{n,k}^m(\eta, \beta)$ is the three-parametric Fermi integral:

$$I_{n,k}^m(\eta, \beta) = \int_0^\infty \frac{e^{x-\eta} x^m (x + \beta x^2)^n}{(1 + e^{x-\eta})^2 (1 + 2\beta x)^k} dx, \quad (2)$$

where $\eta = \mu/k_B T$, $\beta = k_B T/E_g$, T is the temperature, E_g is a band gap, μ is the chemical potential, which could be defined as:

$$\mu = \frac{k_B}{e} T \cdot \ln \left(\frac{N_v}{n} \right), \quad (3)$$

$$N_v = 2 \left(\frac{2\pi m^* k_B T}{h^2} \right)^{\frac{3}{2}}, \quad (4)$$

where N_v is the density of states, m^* is the effective mass, h is Planck's constant and n is the concentration of electrons.

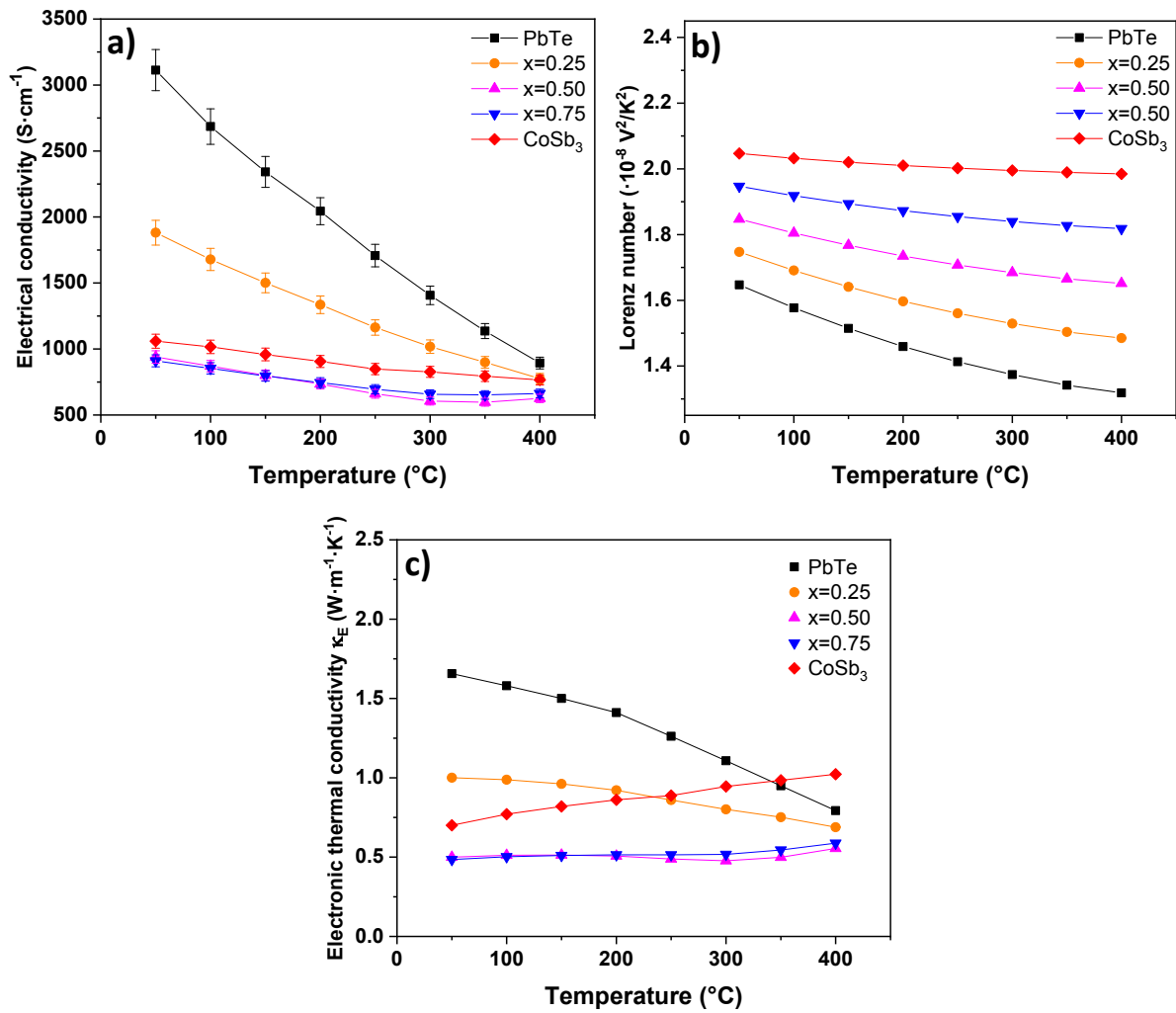


Figure S2. a) Electrical conductivity b) Lorenz number and c) electronic thermal conductivity as a function of temperature in $(1-x)\text{PbTe}/(x)\text{CoSb}_3$ composite for $0 \leq x \leq 1$