Supplementary materials

Thermoelectric performance optimization of n-type $La_{3-x}Sm_xTe_4$/Ni composites via Sm doping

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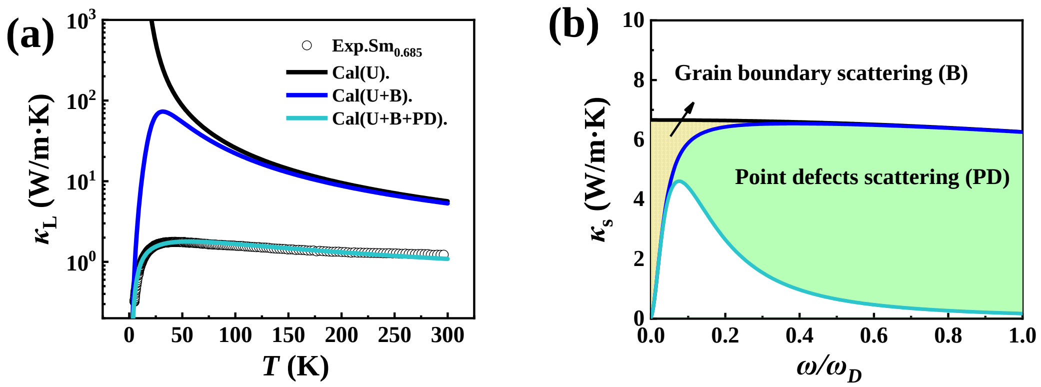

Figure S1. (a) Contribution from various phonon scattering mechanisms to κ_L in $La_{2.315}Sm_{0.685}Te_4$/10 vol.% Ni composite. U, B and PD denote the Umklapp phonon-phonon process, grain boundary scattering and point defect scattering, respectively. (b) Calculated spectral lattice thermal conductivities κ_s for $La_{2.315}Sm_{0.685}Te_4$/10 vol.% Ni composite at 300 K.

Debye-Callaway model for fitting low temperature lattice thermal conductivity

According to the Debye-Callaway model, the lattice thermal conductivity with doping or alloying can be calculated with the following equation [1]:

$$\kappa_L = \frac{k_B}{2\pi^2 v_s}\left(\frac{k_B T}{\hbar}\right)^3 \int_0^{\theta_D/T} \tau_{tot} \frac{z^4 e^z}{(e^z-1)^2} dz \quad \text{(S1)}$$

The integrand item in conjunction with the coefficient of above equation is the spectral lattice thermal conductivity (κ_s), namely:

$$\kappa_s = \frac{k_B}{2\pi^2 v_s}\left(\frac{k_B T}{\hbar}\right)^3 \tau_{tot} \frac{z^4 e^z}{(e^z-1)^2} \quad \text{(S2)}$$

where k_B is the Boltzmann constant, v_s is average sound speed, $\hbar$ is the reduced Plank constant, θ_D is Debye temperature, τ_{tot} is total relaxation time and $z = \hbar\omega/k_B T$ (ω denotes the phonon frequency) is the reduced phonon frequency.

We consider three phonon scattering mechanisms here, including Umklapp phonon-phonon scattering, grain boundary scattering and point defect scattering, which are given by:

$$\tau_{tot}^{-1} = \tau_U^{-1} + \tau_B^{-1} + \tau_{PD}^{-1} \quad \text{(S3)}$$

Umklapp phonon-phonon scattering [2]:

$$\tau_U^{-1} = \frac{\hbar\gamma^2}{\overline{M} v_s^2 \theta_D} \omega^2 T \exp\left(-\frac{\theta_D}{3T}\right) \quad \text{(S4)}$$

Grain boundary scattering:

$$\tau_B^{-1} = \frac{v_s}{G} \quad \text{(S5)}$$

Point defect scattering [3-5]:

$$\tau_{PD}^{-1} = \frac{\overline{V}\omega^4}{4\pi v_s^3} \Gamma \quad \text{(S6)}$$

where γ is the Gruneisen parameter, θ_D is the Debye temperature, v_s is average sound speed, $\overline{M}$ is the average atomic mass, $\overline{V}$ is the average atomic volume, Γ is the disorder scattering parameter, G is the average grain size. The overall phonon scattering relaxation time is expressed as:

$$\tau_{tot}^{-1} = \frac{v_s}{G} + A\omega^4 + B\omega^2 T e^{-\frac{\theta_D}{3T}} \quad \text{(S7)}$$

where A, B are the fitting parameters for point defect scattering, Umklapp phonon-phonon scattering, respectively. The fitting results are shown in Table S1.

Table S1. Fitting results obtained by Debye-Callaway model.

Composition	v_s/G (10^9 s^{-1})	A (10^{-41} s^3)	B (10^{-18} s K^{-1})	R^2	χ^2
$La_{2.315}Sm_{0.685}Te_4$ / 10 vol.% Ni	2.425	4.72	6.452	0.99	0.05

References

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