ELECTRONIC SUPPLEMENTARY INFORMATION FOR

High thermoelectric performance of rapidly microwave-synthesized $Sn_{1-\delta}S$

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Pisarenko line and Lorenz number

Assuming that the dominant mechanism of charge carrier scattering is by acoustic phonons, one obtains the following equations for Seebeck coefficient and carrier density [1]:

$$S = \frac{k_B}{e}\left[\frac{2F_1(\eta)}{F_0(\eta)} - \eta\right] \tag{1}$$

$$n = 4\pi\left(\frac{2m^* k_B T}{h^2}\right)^{3/2} F_{1/2}\,(\eta) \tag{2}$$

Where k_B is the Boltzmann's constant, e is the elementary charge, T is the absolute temperature, m^* is the effective mass, h is the Planck constant, η is the reduced Fermi energy (electrochemical potential), and $F_j(\eta)$ is the Fermi integral:

$$F_j(\eta) = \int_0^\infty \frac{\epsilon^j\, d\epsilon}{1 + \exp(\epsilon - \eta)} \tag{3}$$

Theoretical curves are generated by calculating S versus η, and n versus η. From that data, the Pisarenko relation, S versus n, can be represented.

The total thermal conductivity (κ) is the sum of electronic thermal conductivity (κ_e) and lattice thermal conductivity (κ_l), and can be written in this way:

$$\kappa_l = \kappa - \kappa_e = \kappa - L\sigma T$$

Where L is the Lorenz number, σ is the electrical conductivity and T is the absolute temperature.

Finally, the Lorenz number can be calculated using the expression:

$$L = \frac{{k_B}^2}{e^2}\frac{3F_0(\eta)F_2(\eta) - 4F_1(\eta)^2}{F_0(\eta)^2}$$

Modeling of lattice thermal conductivity

In 1959, J. Callaway proposed a phenomenological model about the lattice thermal conductivity [2], which can be expressed as:

$$\kappa_l = \frac{k_B}{2\pi^2 v}\left(\frac{k_B T}{\hbar}\right)^3 \int_0^{\Theta_D/T} \frac{x^4 e^x}{\tau^{-1}(e^x - 1)^2} dx \quad (4)$$

Where $x = \hbar\omega/k_B T$ is the reduced phonon frequency, k_B is the Boltzmann constant, $\hbar$ is the reduced Planck constant, Θ_D is the Debye temperature, v is the sound velocity, and τ is the effective relaxation time. In this work, τ is expressed as follows [3]:

$$\tau^{-1} = A\omega^4 + B\omega^2 T\, e^{-\Theta_D/3T} + \frac{v}{d} + C\omega^2 \quad (5)$$

Where d is the grain size and v/d represents boundary scattering. A is the pre-factor of point defect scattering relaxation time, B is the prefactor of phonon-phonon Umklapp scattering relaxation time, and C is the prefactor of electron-phonon scattering relaxation time. Some of these parameters can be found in literature [4], and the rest of them can be obtained through fitting the prediction result to the experimental lattice thermal conductivity values.

Table S1 - The parameters used for calculation of the lattice thermal conductivity prediction of SnS sample.

Parameter	Value
A (10^{-42} s^3)	1.88
B (10^{-17} s/K)	3.57
Debye temperature $\boldsymbol{\Theta_D}$ (K)	270
Sound velocity $\boldsymbol{v}$ (m/s)	2424
Average grain size $\boldsymbol{\Theta_D}$ (μm)	10
C (10^{-16} s)	2

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