Electronic Supplementary File for

Transport properties of polycrystalline SnTe prepared by saturation annealing

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Content

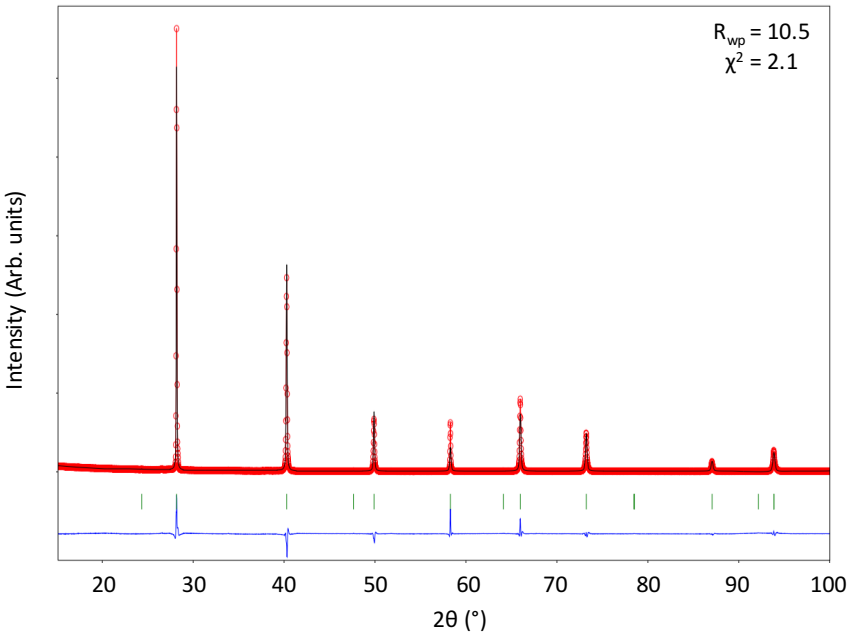

Figure S1. Rietveld refinement against the PXRD data collected on the saturation-annealed sample at 823 K. The experimental data are shown in red, the theoretical pattern in black and the difference curve in blue. The vertical green ticks mark the position of the reflections.

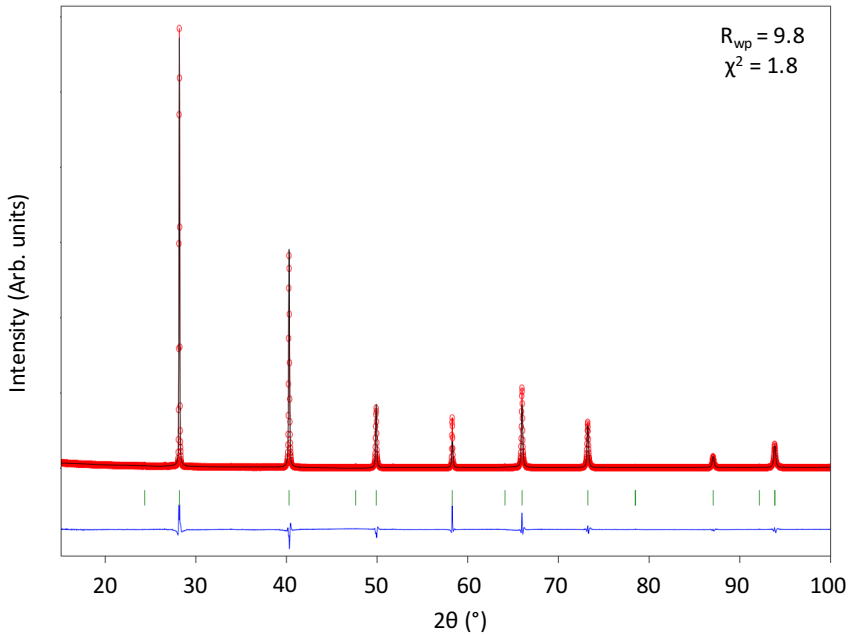

Figure S2. Rietveld refinement against the PXRD data collected on the saturation-annealed sample at 873 K. The experimental data are shown in red, the theoretical pattern in black and the difference curve in blue. The vertical green ticks mark the position of the reflections.

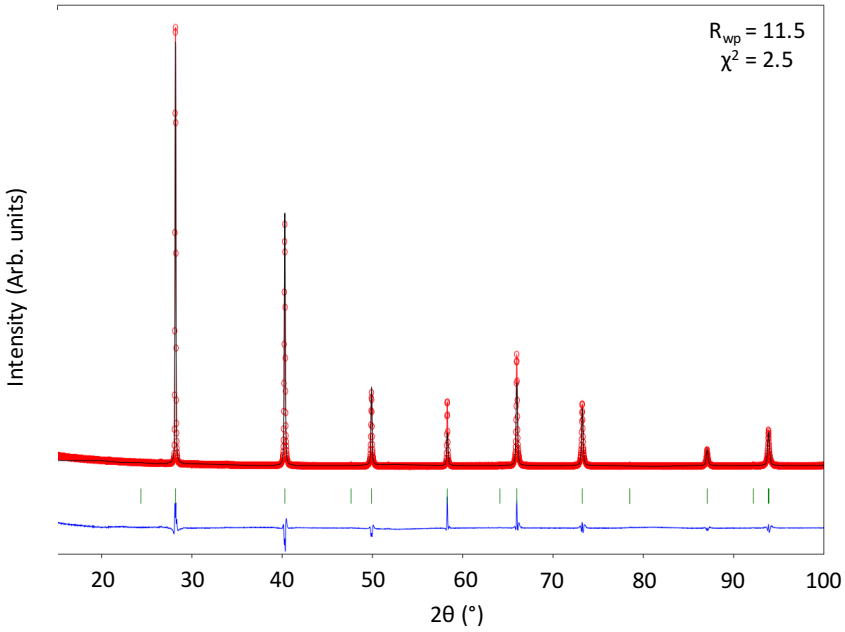

Figure S3. Rietveld refinement against the PXRD data collected on the saturation-annealed sample at 973 K. The experimental data are shown in red, the theoretical pattern in black and the difference curve in blue. The vertical green ticks mark the position of the reflections.

Equations for the Debye-Callaway model used to fit the lattice thermal conductivity of the three saturation-annealed samples

The modeling of the lattice thermal conductivity of the $Sn_{1+x}Te$ samples is based on the expression derived from the Debye model in which the normal processes are neglected. Within this model, the lattice thermal conductivity is expressed as:

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

where $\tau(x,T)$ is the total relaxation time of phonons, $x = \hbar\omega/k_B T$ is a dimensionless parameter, θ_D is the Debye temperature and ω is the phonon pulsation. Following the Matthiessen's rule, the expression for $\tau(x,T)$ can be written as:

$$\tau^{-1} = \frac{v}{L} + A\omega^4 + B\omega^2 T e^{-\theta_D/3T}$$

where L is the average grain size and A and B are adjustable parameters. The first term corresponds to the grain boundary scattering, the second term reflects point-defect scattering and the last term represents phonon-phonon scattering via Umklapp processes.