A combined experimental and modelling approach for the evaluation of the thermoelectric properties of Ag-doped SnS

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S1. Supplementary Figures and Tables



Figure S1. Convergence of the total energy of the pristine SnS model with respect to plane-wave cutoff (a) and k-point sampling (b).



Figure S2. Optimised structure of *Pmcn* SnS shown along the a (a), b (b) and c axes (c). These images were generated using VESTA software.¹



Figure S3. SEM image of the 2.78% sample and EDX spectra showing the atomic composition of the two marked areas. (c) corresponds to a Ag-rich area consistent with the Ag_2SnS_3 secondary phase identified in the XRD measurements.



Figure S4. Total and atom-projected (partial) density of states of the pristine SnS (a/b) and 2.78% Agdoped models (c/d) calculated at the PBEsol (a/c) and HSE06 (b/d) levels of theory.



Figure S5. Calculated temperature-dependent Lorenz number L for the SnS and Ag-doped SnS samples obtained from Equation (9) in the main text.²



Figure S6. Temperature-dependent thermal diffusivity D of the SnS and Ag-doped SnS samples.



Figure S7. Temperature-dependent out-of-plane total thermal conductivity $\kappa(||)$, i.e. parallel to pressing direction, for the SnS and Ag-doped SnS samples.

Samples	Density $(g/cm^3 \pm 3\%)$	Relative density (%)
SnS	5.09	93.1
0.78%	5.08	92.9
1.56%	4.90	89.7
2.78%	4.94	90.5

Table S1. Density and relative density of the SnS and Ag-doped SnS samples.

Table S2. Average grain sizes of the SnS and Ag-doped SnS samples estimated by the line-intercept

 method.

Grain size (μ m	
SnS	0.7
0.78%	0.8
1.56%	2.8
2.78%	3.7

Sample _		Atom %		Actual Ag contents (x)
	Sn	S	Ag	at.%
SnS	49.9 ± 0.1	50.1 ± 0.1		
0.78%	51.5 ± 0.3	48.2 ± 0.3	0.3 ± 0.1	0.6 ± 0.2
1.56%	49.1 ± 0.9	50.2 ± 1.0	0.7 ± 0.1	1.4 ± 0.4
2.78%	49.4 ± 1.1	49.3 ± 0.9	1.3 ± 0.2	2.6 ± 0.7

 Table S3. Sample compositions (atomic ratios and actual Ag content) of the SnS and Ag-doped SnS samples measured using EDX.

S2. Supplementary Methods: Calculation of the In-Plane Thermal Conductivity

The in-plane thermal conductivity $\kappa(\perp)$, i.e. perpendicular to the SPS pressing direction, was estimated from the out-of-plane measurements, i.e. parallel to the SPS pressing direction $\kappa(||)$, based on the ratio $\kappa(||)/\kappa(\perp)$ obtained in other experiments on SnS ceramics.³⁻⁵ As shown in Figure S8, the $\kappa(||)/\kappa(\perp)$ ratio ranges from 0.62 to 0.83, suggesting that the anisotropy falls within this range.⁶ Using the average $\kappa(||)/\kappa(\perp) = 0.73$, we estimated the in-plane κ from our measurements of the out-ofplane κ , and the results are shown in Figure S9.



Figure S8. Ratios of the lattice thermal conductivity κ_L measured parallel and perpendicular to the SPS pressing direction, $\kappa(||)/\kappa(\perp)$, for SnS ceramics prepared in previous studies.³⁻⁵



Figure S9. Estimated in-plane total thermal conductivity κ and lattice thermal conductivity κ_L for SnS, 0.78%, 1.56% and 2.78% ceramic samples.

S3. Supplementary Methods: Electrical-Transport Calculations

Electronic-structure calculations were used to model the electrical-transport properties, *viz.* the Seebeck coefficient *S*, electrical conductivity σ , power factor $S^2\sigma$ (PF) and electronic thermal conductivity κ_e , using semi-classical Boltzmann transport theory within the constant relaxation time approximation (CRTA), as implemented in the AMSET code.⁷

The spectral conductivity tensors $\Sigma_{\alpha\beta}(i, k)$ for an electronic state with band index *i* and wavevector *k* are determined from:

 $\Sigma_{\alpha\beta}(i,k) = e^2 v_{\alpha}(i,k) v_{\beta}(i,k) \tau(i,k) \# (S3.1)_{\text{where}} v(i,k) \text{ and } \tau(i,k) \text{ are the electron group}$ velocities and relaxation times, respectively, and e is the elementary charge. Energy-projected conductivity tensors $\sigma_{\alpha\beta}(E)$ can be obtained by summing over i and averaging over k:

$$\Sigma_{\alpha\beta}(E) = \frac{1}{N} \sum_{i,k} \Sigma_{\alpha\beta}(i,k) \frac{\delta(E - E_{i,k})}{dE} \#(S3.2)$$

where *N* is the number of wavevectors in the summation

and $E_{i, k}$ are the electronic band energies. The σ , S and κ_e and can then be calculated from:^{7,8}

$$\sigma_{\alpha\beta}(T;\mu) = \frac{1}{\Omega} \int \Sigma_{\alpha\beta}(E) \left[-\frac{\partial f(E;\mu,T)}{\partial E} \right] dE \#(S3.3)$$

$$S_{\alpha\beta}(T;\mu) = \frac{1}{eT\Omega} \sigma_{\gamma\alpha}^{-1} \times \int \Sigma_{\gamma\beta}(E)(\varepsilon-\mu) \left[-\frac{\partial f(E;\mu,T)}{\partial E} \right] dE \#(S3.4)$$

$$\kappa_{\alpha\beta}(T;\mu) = \frac{1}{e^2T\Omega} \int \Sigma_{\gamma\beta}(E)(E-\mu)^2 \left[-\frac{\partial f(E;\mu,T)}{\partial E} \right] dE \#(S3.5)$$

where μ is the chemical potential (equal to the Fermi energy E_F for a given doping level), Ω is the cell volume and f is the Fermi-Dirac distribution function given by:

$$f(E,\mu,T) = \frac{1}{exp[(E-\mu)/k_BT] + 1} \#(S3.6)$$

where k_B is the Boltzmann constant.

In the CRTA model the $\tau(i,k)$ in Eq. (S3.1) are treated as a (single) unknown constant τ_e . The Seebeck coefficient is in principle independent of this parameter, as it is the ratio of two spectral conductivity tensors, whereas the conductivity and electrical thermal conductivity are obtained divided by this constant, i.e. as σ/τ_e and κ/τ_e .

The transport calculations require as their main input a high-quality uniform electronic bandstructure calculation with a dense k-point sampling, i.e. a set of band energies $E_{i,k}$ and corresponding Kohn-Sham orbitals, which are used to calculate the v(i, k). Based on this, the transport coefficients are determined for a specified set of extrinsic carrier concentrations ("doping levels") n, which determine the $\mu = E_F$, temperatures, and an electron relaxation time τ_e .

k-point convergence tests were performed on the pristine SnS model using PBEsol, with nominal values of $n = 10^{16}$ and 10^{19} cm⁻³, temperatures from 300-800 K, and a constant $\tau_e = 4.06 \times$ 10^{-15} s estimated from experiments (Figure S10).^{4, 9, 10} These tests indicated that using 2-3 × denser *k*-point meshes than the "base" mesh used for the geometry optimisation during the electronicstructure calculation, and enhancing these by a further 5 × using interpolation during the transport calculations, was sufficient to converge the calculated transport properties.

The intrinsic n can be estimated from the calculated electronic density of states g(E) (DoS) according to:

$$n(T) = \int_{E_F}^{\infty} f(E,\mu = E_F,T)g(E)dE\#(S3.7)$$

Figure S11 shows the calculated PBEsol DoS of pristine SnS with the $f(E,\mu,T)$ at T = 300 and 800 K. The intrinsic *n* were calculated using this method for a series of temperatures from 300-800 K, and used in transport calculations to test two further technical parameters.

Firstly, we compared the effect of using two Sn pesudopotentials (PPs), "Sn_d" and "Sn", the latter of which subsumes the semi-core Sn 4d states into the core and thereby halves the number of valence electrons per SnS formula unit that need to be treated in the calculations. As shown in Figure S12, the two PPs yield very similar DoS curves, calculated n, mobilities μ and electrical conductivities σ , for both the base and $2/3 \times k$ -point sampling meshes, but yielded markedly different S and hence power factors $S^2\sigma$ with smaller k-point sampling. Based on these tests, we determined that using the cheaper "Sn" PP, without semi-core states, together with the $2 \times k$ -sampling chosen from the convergence tests, is a reasonable approximation.

Having established this, we then checked the convergence of more accurate HSE06 hybrid calculations, using the "Sn" PP, with respect to k-point sampling. Even with fewer valence electrons per formula unit, the much larger computational cost of calculations with hybrid functionals means that we were only able to test the "base" and 2 × denser sampling. We therefore also performed non self-consistent calculations,¹¹ where the HSE06 eigenvalues are calculated from PBE Kohn-Sham orbitals without self-consistent orbital updates, to access up to 3 × denser k-point sampling. As shown in Figure S13, we found that the non self-consistent HSE06 calculations gave similar results to the self-consistent calculations, and confirmed that the 2 × k-point sampling found to converge the PBEsol transport calculations was also sufficient to converge the HSE06 calculations.

To attempt to compare to the experimental data, transport calculations were performed at each of the experimental measurement temperatures over a range of $n = 10^{15} - 10^{20}$ cm⁻³ and the S, σ and κ_e compared to the measured values (Figure S14). Within the CRTA the S are independent of the relaxation time τ_e . Comparison of the measured S with the predicted S(n) therefore allows a set of n to be determined that best reproduce the S at each of the measurement temperatures. The σ obtained

from the CRTA are scaled by the τ_e . The ratio of the σ obtained with the fitted n and the measured σ can thus be used to determine a scale factor for the initial τ_e to derive a fitted relaxation time. We therefore obtain, for each measurement temperature, a fitted n and τ_e that reproduce the measured S and σ (and hence PFs). The mobility and κ_e with the fitted parameters can also be obtained.

Figure S15 compares the fitted S and σ to the experimental measurements. Both variants of HSE06 can reproduce the measured S with a suitable value of n, and the σ with the fitted n and a scaled τ_e . On the other hand, the PBEsol calculation is not able to reproduce the S, which makes the fitted parameters somewhat questionable. We attribute this to the underestimated bandgap and consequent larger intrinsic n obtained with PBEsol.

Convergence tests with PBEsol on the three doped models indicated that $2 \times \text{denser } k$ -point meshes were appropriate for the smaller 1.56% and 2.78% models, whereas a $3 \times \text{denser mesh}$ was required for the largest 0.78% model due to the small base mesh used for this system. Due to the size of the doped models, it was not practical to perform HSE06 calculations with the converged k-point meshes. However, we found that, as for pristine SnS, transport calculations with PBEsol would be unable to reproduce the measured S. Given that the Fermi energy in these models lies within the valence band, this is most likely due to the imposed hole concentration being much higher than achieved in the experiments, and the same issue would occur with HSE06 electronic-structure calculations. As described in the text, we therefore opted to use the (self-consistent) HSE06 calculation on pristine SnS with the $2 \times \text{denser } k$ -point mesh to analyse all three experimental samples.



Figure S10. Predicted σ , S and κ_e of pristine SnS as a function of temperature, with two doping levels of $n = 10^{16}$ and 10^{19} cm⁻³ and a constant $\tau_e = 4.06 \times 10^{-15}$ s,^{4, 9, 10} obtained from PBEsol electronicstructure and transport calculations with up to 5 × denser *k*-point sampling compared to the "base" mesh used for the geometry optimisations.



Figure S11. Calculated electronic density of states g(E) (DoS) of pristine SnS obtained with the PBEsol functional (2 × *k*-point sampling), with the Fermi-Dirac distribution in Equation (S3.6) at T = 300 and 800 K overlaid for comparison.



Figure S12. Comparison of the predicted carrier concentration n (a), mobility μ (b), electrical conductivity σ (c), Seebeck coefficient S (d), power factor $S^2\sigma$ (PF, e) and electrical thermal conductivity κ_e (f) obtained from electronic-structure and transport calculations with PBEsol and up to $3 \times k$ -point sampling, and Sn pseudopotentials with the semi-core Sn 4d electrons in the core ("Sn") and valence regions ("Sn_d").



Figure S13. Comparison of the predicted carrier concentration n (a), mobility μ (b), electrical conductivity σ (c), Seebeck coefficient S (d), power factor $S^2\sigma$ (PF, e) and electrical thermal conductivity κ_e (f) as a function of temperature obtained from electronic-structure and transport calculations with HSE06 and non-self-consistent ("NSC") HSE06 and up to $3 \times k$ -point sampling.



Figure S14. Predicted electrical conductivity σ (a), Seebeck coefficient S (b) and electronic thermal conductivity κ_e of pristine SnS as a function of doping level n and temperature, obtained from electronic-structure and transport calculations with HSE06 (2 × k-point sampling), compared to experimental measurements.



Figure S15. Comparison of the predicted concentration n (a), mobility μ (b), electrical conductivity σ (c), Seebeck coefficient S (d), power factor $S^2\sigma$ (PF, e) and electrical thermal conductivity κ_e (f) as a function of temperature to experimental measurements. Three sets of predictions are shown, based on electronic-structure and transport calculations with PBEsol (3 × k-point sampling), HSE06 (2 × k-point sampling) and non-self-consistent ("NSC") HSE06 (3 × k-point sampling), in each case with fitted n and electron relaxation times τ_e as described above.

S4. Supplementary Methods: Calculation of Lattice Thermal Conductivity

Computing the lattice-thermal conductivity κ_L requires calculation of the second-order force constants (FC2), which are used to calculate the phonon heat capacities C_{λ} and group velocities ν_{λ} in Equation (3) in the text, and the third-order force constants (FC3), which are combined with the harmonic phonon frequencies and eigenvectors to determine the phonon lifetimes $\tau_{\lambda,12}$ Both the FC2 and FC3 are determined using finite differences by calculating the change in forces in response to small displacements of the symmetry-independent atoms in an appropriate supercell. Once the FC2 and FC3 have been calculated, the modal properties must then be determined on an appropriate grid of reciprocal-space phonon wavevectors (*q*-points) to sample the phonon Brillouin zone.

The κ_L of pristine SnS was calculated using 4×4×2 and 3×3×1 supercell expansions (256/72 atoms) to determine the FC2 and FC3 and a 16×16×8 q-point mesh, all of which are in line with our previous studies.^{13, 14}

Given the different supercells used to create the three Ag-doped models, it was not possible to select a common supercell expansion for computing the FCs. The FC2 of the smaller 2.78% model were computed in a $1 \times 1 \times 2$ supercell expansion, equivalent to a $3 \times 3 \times 2$ supercell of pristine SnS (144 atoms), while the FC2 of the larger models were computed in supercells equivalent to a $4 \times 4 \times 2$ supercell of SnS (256 atoms). To confirm the harmonic properties from both supercells were converged, we compared phonon density of states (DoS) and dispersion curves of pristine SnS computed with FC2 determined using $3 \times 3 \times 2$ and $4 \times 4 \times 2$ supercells and found that both yielded practically identical results (Figure 16).

Due to the symmetry lowering induced by the Ag for Sn substitution, the number of displacements required to compute the FC3 in a single cell of the 2.78% model, which is based on the same $3 \times 3 \times 1$ expansion used to calculate the FC3 of pristine SnS, was impractical. We therefore applied

a 5 Å cutoff in order to limit the number of calculations. The calculated κ_L of pristine SnS with the same cutoff imposed to the FC3 gave very similar results to those obtained with the full set of FCs (Figure S17), suggesting this approximation is reasonable. We also calculated the κ_L using the smaller $3\times3\times2$ FC2 SC, with and without the range cutoff, and again found similar results, which further supports the similar phonon spectra in Figure S16.

For similar reasons, it was not possible to calculate the FC3 of the larger 0.78% and 1.56% models, even with a range cutoff. For these systems, we instead adapted the approximate model developed in our previous work on alloys.¹⁴ In the SM-RTA model, the FC3 are required to calculate the three-phonon interaction strengths $\Phi_{\lambda\lambda'\lambda''}$ to obtain the phonon lifetimes. If these can be replaced by a suitable constant value \mathcal{P} , the κ_L can be estimated from a harmonic phonon calculation. Suitable weighted average values of the $\Phi_{\lambda\lambda'\lambda''}$ were determined as described in our previous work from a linear fit of the κ_L as a function of \mathcal{P}^{-1} to determine the \mathcal{P} that reproduce the calculated κ_L of the pristine SnS and 2.78% models at a reference temperature of 600 K (Figure S18 and S19).

Noting that the P need to be scaled by $(3n_a)^2$ to compare between systems, where n_a is the number of atoms in the primitive unit cell and there are therefore $3n_a$ bands at each q-point,¹⁵ the scaled $P = 2.95 \times 10^{-8}$ and 3.91×10^{-8} obtained for the SnS and 2.78% models at 600 K differ by ~30%. The value for SnS at 300 K is 14% larger than value of 2.52×10^{-8} eV² obtained in our previous work, which included a dispersion correction.¹⁴ As a test, we calculated the κ_L of the 2.78% model using the (rescaled) P for pristine SnS, and obtained a reasonable estimate of the κ_L of each of the 0.78% and 1.56% models, and interpolated between them based on the Ag doping concentration (Figure S21 and S22).

The predicted κ_L for all three doped models were found to be very low in comparison to the experimental measurements. Solving the phonon Boltzmann transport equation (BTE; here within the SM-RTA) accounts for the contribution to the κ_L from "particle-like" transport. However, in materials where dense band structures and/or broad phonon linewidths cause bands to overlap, there is an additional contribution to the κ_L from "wave like" tunnelling of energy between modes. Both the particle-like and wave-like contributions $\kappa_L = \kappa_P + \kappa_W$ can be computed by solving the Wigner transport equation (WTE).¹⁶ As shown in Figures S23-26, we find that the κ_W terms for the doped models are comparable to the κ_p between ~100-200 K and significantly larger than the κ_p at high temperature, and also that the κ_W also makes a smaller but non-negligible contribution to the κ_L of pristine SnS at high T. Furthermore, while the κ_P of the three doped models is similar, the progressive "unfolding" of the band structure as the supercell size is increased to model lower doping concentrations results in a "denser" band structure, smaller intraband spacing, and larger κ_W , recovering the chemically-intuitive result that the κ_L increases, and converges towards that or pristine SnS, as the doping concentration is reduced. We therefore conclude that to model the κ_L of doped supercell models it is likely insufficient to solve the BTE and consider only the particle-like conductivity, and solving the WTE is necessary in order to account for the wave-like contribution to the κ_L .



Figure S16. Total and atom-projected (partial) phonon density of states (DoS; a/c) and phonon dispersion curves (b/d) of SnS computed using second-order force constants obtained in (a/b) $3 \times 3 \times 2$ and (c/d) $4 \times 4 \times 2$ supercell expansions.



Figure S17. Comparison of the averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ of SnS computed using $3 \times 3 \times 2$ and $4 \times 4 \times 2$ supercell expansions to determine the second-order force constants (FC2) and a $3 \times 3 \times 1$ expansion to determine the third-order force constants (FC3) and with and without a 5 Å cutoff range.



Figure S18. Determination of the averaged three-phonon interaction strength \mathcal{P} of pristine SnS. (a) Averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ as a function of \mathcal{P}^{-1} at T = 300, 600and 900 K showing the value of \mathcal{P}^{-1} that reproduces the calculated values. (b) Fitted \mathcal{P} as a function of temperature. (c) Calculated κ_{ave} as a function of temperature obtained with the calculated (permode) interaction strengths and with interaction strengths set to the fitted \mathcal{P} at300, 600 and 900 K.



Figure S19. Determination of the averaged three-phonon interaction strength \mathcal{P} of 2.78% Ag-doped SnS. (a) Averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ as a function of \mathcal{P}^{-1} at T = 300, 600 and 900 K showing the value of \mathcal{P}^{-1} that reproduces the calculated values. (b) Fitted \mathcal{P} as a function of temperature. (c) Calculated κ_{ave} as a function of temperature obtained with the calculated (per-mode) interaction strengths and with interaction strengths set to the fitted \mathcal{P} at300, 600 and 900 K.



Figure S20. Comparison of the averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ of 2.78% Ag-doped SnS computed with the calculated (per-mode) three-phonon interaction strengths, with a 5 Å cutoff applied to the third-order force constants, and with the rescaled constant interaction strength P determined for pristine SnS.



Figure S21. Comparison of the averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ of 0.78% Ag-doped SnS computed with the rescaled constant interaction strengths P determined for pristine and 2.78% Ag-doped SnS together with κ_{ave} determined by interpolating between the two curves based on the doping concentration.



Figure S22. Comparison of the averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ of 1.56% Ag-doped SnS computed with the rescaled constant interaction strengths P determined for pristine and 2.78% Ag-doped SnS together with κ_{ave} determined by interpolating between the two curves based on the doping concentration.



Figure S23. Averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ of pristine SnS computed by solving the Wigner transport equation (WTE). The total thermal conductivity $\kappa_L = \kappa_P + \kappa_W$ (orange) is shown together with the particle-like and wave-like contributions κ_P (blue) and κ_W (red). This calculation is performed with the second-order force constants determined in a 4×4×2 supercell expansion of the *Pnma* SnS unit cell.



Figure S24. Averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ of 2.78% Ag-doped SnS computed by solving the Wigner transport equation (WTE). The total thermal conductivity $\kappa_L = \kappa_P + \kappa_W$ (orange) is shown together with the particle-like and wave-like contributions κ_P (blue) and κ_W (red). This calculation is performed with the third-order force constants determined with a 5 Å cutoff.



Figure S25. Averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ of 1.56% Ag-doped SnS computed by solving the Wigner transport equation (WTE). The total thermal conductivity $\kappa_L = \kappa_P + \kappa_W$ (orange) is shown together with the particle-like and wave-like contributions κ_P (blue) and κ_W (red). This calculation is performed with the rescaled constant interaction strengths \tilde{P} interpolated between the pristine SnS and 2.78% Ag-doped SnS models.



Figure S26. Averaged lattice thermal conductivity $\kappa_{ave} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ of 0.78% Ag-doped SnS computed by solving the Wigner transport equation (WTE). The total thermal conductivity $\kappa_L = \kappa_P + \kappa_W$ (orange) is shown together with the particle-like and wave-like contributions κ_P (blue) and κ_W (red). This calculation is performed with the rescaled constant interaction strengths \tilde{P} interpolated between the pristine SnS and 2.78% Ag-doped SnS models.

S5. Supplementary Methods: Calculation of Lotgering Factors

The degree of preferred orientation was determined from the XRD data using the Lotgering factor, LF:¹⁷

 $LF = \frac{p - p_0}{1 - p_0} \#(S5.1)$ where *p* and *p*₀ are calculated using the peak intensities from the measured and

reference patterns respectively. For example, p and p_0 of (*hk*4) plane can be calculated as follows:

$$p = \frac{\sum_{hk}^{I} (hk4)}{\sum_{hkl}^{I} (hkl)} \#(S5.2)$$
$$p_{0} = \frac{\sum_{hk}^{I} I_{0} (hk4)}{\sum_{hkl}^{I} I_{0} (hkl)} \#(S5.3)$$

The LF ranges from 0 to 1, indicating random and perfect orientation respectively. The calculated LFs for the (11l) and (hk4) planes parallel and perpendicular to the pressing direction are shown in Table S4.

Table S4. Lotgering factors (LFs) measured for the (11*l*) and (*hk*4) planes parallel (||) and perpendicular (\perp) to the pressing direction.

	∥ (11 <i>l</i>)	$\perp (hk4)$
SnS	0.124	0.282
0.78%	0.085	0.290
1.56%	0.096	0.276
2.78%	0.075	0.526

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