Synthesis of High-Density Bulk Tin Monoxide and Its Thermoelectric Properties

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SnSe exhibits exceptionally high thermoelectric (TE) figure of merit zT mainly due to its ultralow lattice thermal conductivity (κ_{lat}) [L.-D. Zhao *et al.*: Nature **508** (2014) 373.]. It is considered that strong lattice anharmonicity caused by the lone pair electrons of Sn^{2+} results in the ultralow κ_{lat} . Here, we focus on SnO because it has the lone pair electrons of Sn^{2+} like SnSe. Bulk samples of SnO were synthesized by low-temperature high-pressure spark plasma sintering and their TE properties were examined. The present study revealed that SnO exhibits very low κ_{lat} ($1.44 \text{ W m}^{-1} \text{ K}^{-1}$ at 573 K) compared with SnO_2 which has no lone pair electrons. The Grüneisen parameter (γ) of SnO was evaluated to be 1.70 and this high γ leads to large lattice anharmonicity and thereby low κ_{lat} . Even though SnO has low κ_{lat} , the zT values were significantly low compared with SnSe. The maximum zT value of SnO was 0.00141 at 573 K. Since the main reason of this low zT is its non-optimized carrier concentration, the zT of SnO can be enhanced through the carrier concentration optimization. [doi:10.2320/matertrans.E-M2018804]

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1. Introduction

Thermoelectric (TE) materials can convert heat into electricity and vice versa. The conversion efficiency of TEs is mainly determined by the materials' properties called dimensionless figure of merit, $zT = S^2 \sigma T / \kappa$, where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature, and κ is the total thermal conductivity ($\kappa = \kappa_{\text{lat}} + \kappa_{\text{el}}$, sum of the contributions from lattice and electronic).¹⁾ Thus, to enhance the zT , high electrical properties, i.e. high $S^2 \sigma$, as well as low κ are required. Since there exists a trade-off relationship among S and σ or κ_{el} depending on the carrier concentration, the most effective way to enhance zT is the reduction of κ_{lat} , which is nearly independent of the carrier concentration.

The reduction of κ_{lat} with keeping high electrical properties has been demonstrated in many TE materials, including filled-skutterudites^{2–4)} and nanostructured materials.^{5–10)} In the filled-skutterudites, AM_4X_{12} , the A atoms called filler elements are bonded weakly to the other atoms and rattles, leading to strong scattering of phonons, resulting in low κ_{lat} .¹¹⁾ In the nanostructured materials, the nanoscale intermediates scatter phonons much more effectively than carriers, when the size of the structure is smaller than the phonon mean free path but larger than the carrier mean free path, leading to a reduction in κ_{lat} without a negative effect on the electrical properties.^{12,13)} On the other hand, a new concept of lattice anharmonicity to reduce κ_{lat} has been proposed recently.^{14–20)} For example, an extremely low κ_{lat} ($0.23 \pm 0.03 \text{ W m}^{-1} \text{ K}^{-1}$ at 973 K) was obtained in SnSe,²¹⁾ and it has been considered that this significantly reduced κ_{lat} is mainly due to the high rate of lattice anharmonicity induced by the lone pair electrons of Sn^{2+} . This anharmonicity is driven by a stereochemically active lone pair electrons produced by the interaction between Sn ($5p$)

and antibonding Sn ($5s$)-X (p) states.²²⁾ Owing to this quite low κ_{lat} , SnSe exhibits record-high zT value of 2.6 ± 0.3 at 923 K.²¹⁾ However, despite having very high zT , usability of SnSe is limited by several disadvantages of using Se, because Se is highly toxic and small production scale.^{23,24)}

Here, we focus on SnO which has lone pair electrons of Sn^{2+} like SnSe as O is in the same group 16 elements as Se.²²⁾ A fine bulk sample of SnO is hard to be synthesized because SnO is decomposed into SnO_2 and Sn between 700 and 1050 K.²⁵⁾ It is reported that the following disproportionation reactions of SnO occur in a N_2 atmosphere:

This is why the physical properties of bulk SnO have been hardly measured so far. In this paper, we report on the temperature-dependent κ_{lat} and the Grüneisen parameter (γ) at room temperature of SnO and discuss the relationship among the lone pair electrons, anharmonicity, and κ_{lat} . γ can be used as a measure of anharmonicity. For further discussion of the influence of the lone pair electrons on the κ_{lat} , we compared the κ_{lat} and γ values of SnO with those of SnO_2 which has no lone pair electrons. Figures 1(a) and 1(b) show the crystal structures of SnO and SnO_2 , respectively. SnO has a tetragonal structure with the space group $P4/nmm$,²⁶⁾ while SnO_2 has a tetragonal structure with the space group $P4_2/mnm$.²⁷⁾ Unlike SnO_2 with a three dimensional structure, SnO has a layered structure where the lone pair electrons of Sn^{2+}

Fig. 1 Three-dimensional crystal structures of (a) SnO and (b) SnO_2 .

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above the apexes of SnO_4 square-based pyramids reside in the interstitial space between the layers.²⁸⁾ Such a structural feature is expected to be responsible for strong lattice anharmonicity.

2. Experimental Procedure

SnO (200 mesh, 99.9%, Furuuchi Chemical Co. Ltd.) powders were used as raw materials to prepare the bulk samples. To determine the sintering conditions, high-temperature stability of SnO was checked by the thermogravimetry/differential thermal analysis (TG-DTA) measurement both in air and an Ar atmosphere with a heating rate of 20 K min^{-1} . The SnO powders were placed into a tungsten-carbide die, followed by spark-plasma-sintering (SPS) in an Ar flow atmosphere under four different pressure/temperature conditions (#1 500 MPa/573 K, #2 500 MPa/598 K, #3 500 MPa/623 K, and #4 300 MPa/673 K). The powders used for the SPS condition #2 were ball-milled at a rotational speed of 300 rpm for 10 min before the sintering process. In addition to SnO , commercially-available SnO_2 tablets (ϕ 10.0 mm, height 5.0 mm, 99.99%, 88.5% T.D., Kojundo Chemical Laboratory Co., Ltd.) were prepared and their physical properties were characterized to compare the data with those of SnO . The phase state and microstructure of the samples were evaluated at room temperature by powder X-ray diffraction analysis (XRD; Ultima IV, Rigaku Co.) with $\text{Cu K}\alpha$ radiation and scanning electron microscopy (SEM, JSM-6500F, JEOL) equipped with an energy dispersive spectrometer (EDS). κ was calculated by $\kappa = \alpha C_p d$, where α , C_p , and d are the thermal diffusivity, specific heat capacity at constant pressure, and density, respectively. α parallel to the SPS (pressing) direction was measured in the temperature range from room temperature to 673 K in an Ar atmosphere using a light flash apparatus (Netzsch LFA-467). The C_p data were obtained from the literatures.^{29,30)} d was calculated from the measured weight and dimensions of the bulk samples. κ_{lat} was calculated by subtracting κ_{el} from κ , where κ_{el} was estimated by the Wiedemann-Franz law, i.e. $\kappa_{\text{el}} = LT\sigma$ (L is the Lorenz number for nondegenerate limit: $1.5 \times 10^{-8} \text{ W}\Omega\text{K}^{-2}$). The volumetric thermal expansion coefficient (α_v) was evaluated by two methods, high temperature XRD analysis in a He atmosphere and direct measurement using a dilatometer in an Ar flow atmosphere. The α_v perpendicular to the press direction was measured using a dilatometer. The α_v of SnO and SnO_2 were evaluated in the temperature ranges from room temperature to 673 K and 973 K, respectively. The longitudinal (v_l) and transverse speed of sound (v_t) were measured by an ultrasonic pulse-echo method at room temperature in air using 10 MHz sound wave echogenic transducers. These properties were measured in the parallel to the press direction. S and σ of the bulk samples of SnO were simultaneously measured in the temperature range from room temperature to 573 K using a commercial apparatus (Advance Riko ZEM-3) under a He atmosphere. These properties were measured in the perpendicular to the press direction. The Hall coefficient (R_H) was measured by the Van der Pauw technique with a Hall measurement system (Toyo Resitest8300) at room temperature in vacuum under an applied magnetic field of

0.5 T. The Hall carrier concentration (n_H) and Hall mobility (μ_H) were calculated from the expressions $n_H = 1/|R_H|e$ (e : elementary electric charge) and $\mu_H = |R_H|\sigma$, respectively.

3. Results and Discussion

It was confirmed from the XRD analysis that the as-received SnO powders and SnO_2 tablet are single phase materials with no remarkable impurities (Fig. 2). Figures 3(a) and 3(b) show the TG-DTA curves of as-received SnO powders performed in an Ar-flow atmosphere and in air, respectively. As can be seen in Fig. 3(a), SnO exhibits good thermal stability in an Ar-flow atmosphere up to around 1000 K. On the other hand, SnO oxidizes in air at around 700 K. In case of the complete oxidation of SnO to SnO_2 , the mass change is around 12%. However, in the present case, the mass change is only 1.6%, which can be confirmed from the TG curve in Fig. 3(b). This result means that the oxidation occurs only at the surface of the SnO powders and thus SnO_2 layers act as barriers for farther oxidation. From the TG-DTA results, we determined the SPS conditions.

The powder XRD patterns of the bulk samples of SnO synthesized by SPS are shown in Fig. 4, together with the literature data of SnO ,³¹⁾ SnO_2 ,³²⁾ and Sn .³³⁾ It can be confirmed that the samples #1 (573 K, 500 MPa) and #2 (598 K, 500 MPa) are almost pure SnO , while the samples #3 (623 K, 500 MPa) and #4 (673 K, 300 MPa) contain SnO_2 clearly as an impurity phase. At 623 K and above, the sample is stable during the TG-DTA measurement while it

Fig. 2 Powder XRD patterns of as-received SnO powders and SnO_2 tablet, together with the literature data of SnO ³¹⁾ and SnO_2 .³²⁾

Fig. 3 TG-DTA curves of as-received SnO powders, (a) in an Ar-flow atmosphere and (b) in air.

Table 1 Lattice parameters and relative densities of the samples. The literature data of the lattice parameters of $\text{SnO}^{31)}$ and $\text{SnO}_2^{32)}$ are shown for comparison.

		Lattice parameter (nm)		Relative density (%T.D.)
		a	c	
SnO	As-received powders	0.3797 (16)	0.4830 (19)	-
	SPS bulk # 1	0.3788 (12)	0.4832 (17)	85.2
	SPS bulk # 2	0.3795 (10)	0.4824 (14)	90.2
	SPS bulk # 3	0.3795 (15)	0.473 (5)	89.6
	SPS bulk # 4	0.3792 (7)	0.4828 (15)	87.6
	Reference data ³¹⁾	0.38029	0.48382	-
SnO ₂	As-received tablet	0.4726 (3)	0.3183 (2)	88.5
	Reference data ³²⁾	0.47367	0.31855	-

Fig. 4 Powder XRD patterns of the bulk samples of SnO synthesized by SPS and bulk XRD pattern of sample #2 for the perpendicular plane to the SPS (pressing) direction, together with the literature data of $\text{SnO}^{31)}$, $\text{SnO}_2^{32)}$ and $\text{Sn}^{33)}$

decomposes during the SPS process. It has been reported that the decomposition rate of SnO into SnO_2 and Sn remarkably increases under high pressure (2–15 GPa).³⁴⁾ Therefore, the decomposition rate would also increase under the SPS pressure (500 MPa), which leads to the decomposition of the sample during the SPS process. Table 1 summarizes the lattice parameters and densities of the samples. Among the SnO samples, the lattice parameters are slightly different each other, likely due to the slight differences in the O/Sn ratio. The sample #2 exhibits the highest relative density of 90.2%, thus, we used this sample for physical properties measurements. The bulk XRD pattern of sample #2 for the perpendicular plane to the SPS (pressing) direction is shown in Fig. 4. It is confirmed that the intensity of the (002) peak of the bulk sample is slightly higher than that of the powder sample, meaning that the bulk sample is slightly oriented to the [001] direction. Although the bulk sample is slightly

Fig. 5 Appearance of the bulk samples of (a) SnO (sample #2) and (b) as-received SnO_2 tablet.

Fig. 6 SEM and EDX mapping images of (top three images) the bulk sample of SnO (sample #2) and (bottom three images) as-received SnO_2 tablet.

oriented to the [001] direction, the physical properties are evaluated under the assumption that the sample is not anisotropic but isotropic. The appearance of the bulk sample of SnO (sample #2) and as-received SnO_2 tablet is shown in Figs. 5(a) and 5(b), respectively. Due to the difference in the band gap energy (E_g), SnO ($E_g = 0.73 \text{ eV}^{35)}$ is black colored, while SnO_2 ($E_g = 3.64 \text{ eV}^{36)}$ is white. Figure 6 shows SEM images and the EDX mapping images of the bulk sample of SnO (sample #2) and as-received SnO_2 tablet. Both samples are homogeneous and no remarkable cracks and pores. SnO_2 tablet has slightly smaller grains ($< \sim 5 \mu\text{m}$) than those of the SnO bulk sample. The white area in the SEM image of SnO may correspond to SnO_2 existed as the impurity phase.

Figure 7 shows the temperature dependences of the lattice thermal conductivities (κ_{lat}) of SnO and SnO₂. Since σ values of both SnO and SnO₂ are very small, κ_{el} can be neglected, i.e., $\kappa \approx \kappa_{\text{lat}}$. In the present study, the samples contain pores, thus the Maxwell-Eucken equation was adopted for the correction of porosity in κ_{lat} . The equation is expressed as follows:³⁷⁾

$$\kappa_0 = \kappa_P \frac{(1 + \beta P)}{(1 - P)}, \quad (2)$$

where κ_0 is the thermal conductivity with no pores, κ_P is the thermal conductivity of a sample with porosity P , and β is a constant depending on the shape of the pores (here, $\beta = 0.5$ ³⁸⁾). The density-corrected κ_{lat} are plotted along with the measured data. As can be confirmed in Fig. 7, SnO has much smaller κ_{lat} values than SnO₂.

To understand the origin of the low κ_{lat} of SnO compared with SnO₂, the κ_{lat} is analyzed by using various physical properties obtained in the present study. Figure 8 shows the temperature dependences of the lattice parameters and lattice volume of SnO and SnO₂ obtained by the HT-XRD measurement. It can be confirmed that all the parameters of both SnO and SnO₂ increase linearly with increasing temperature. The average linear thermal expansion coefficient (α_L) and the average volumetric thermal expansion coefficient (α_V) are determined by the following equations:

$$\alpha_L = \frac{1}{l_0} \frac{dL}{dT}, \quad (3)$$

$$\alpha_V = \frac{1}{V_0} \frac{dV}{dT}, \quad (4)$$

where l_0 and V_0 are the lattice parameter and lattice volume at room temperature, respectively. The values of α_L along the a -axis (α_a) and c -axis (α_c) and α_V are summarized in Table 2. The α_V of SnO ($9.97 \times 10^{-5} \text{ K}^{-1}$) is clearly larger than that of SnO₂ ($1.89 \times 10^{-5} \text{ K}^{-1}$), showing that larger anharmonicity of SnO than that of SnO₂. As for SnO, the α_c ($5.21 \times 10^{-5} \text{ K}^{-1}$) is larger than the α_a ($2.33 \times 10^{-5} \text{ K}^{-1}$), which is consistent with the fact that SnO is bounded by a strong

Fig. 7 Temperature dependence of the lattice thermal conductivity (κ_{lat}) of the bulk sample of SnO (sample #2) and as-received SnO₂ tablet. Density-corrected data are shown in lines.

Fig. 8 Temperature dependences of the lattice parameters a and c , and lattice volume V of SnO (top three figures) and SnO₂ (bottom three figures).

Table 2 Linear thermal expansion coefficient along the a -axis α_a , linear thermal expansion coefficient along the c -axis α_c , linear thermal expansion coefficient α_L , volumetric thermal expansion coefficient α_V , longitudinal speed of sound v_l , transverse speed of sound v_t , average speed of sound v_m , Debye temperature θ_D , bulk modulus B , and Grüneisen parameter γ of SnO and SnO₂. The thermal expansion data are the average values in the temperature range between 300 and 700 K for SnO and 300 and 1000 K for SnO₂. The data of the speed of sound are the density-corrected ones. The literature data for SnO₂^{32,42,43)} are shown for comparison.

	SnO	SnO ₂	Remarks
α_a (K ⁻¹)	2.33×10^{-5}	6.14×10^{-6}	Evaluated by temperature dependence of the lattice parameters obtained from the high-temperature XRD analysis
α_c (K ⁻¹)	5.21×10^{-5}	6.58×10^{-6}	
α_V (K ⁻¹)	9.97×10^{-5}	1.89×10^{-5}	
α_L (K ⁻¹)	1.86×10^{-5}	5.87×10^{-6}	Measured directly by using a dilatometer
α_V (K ⁻¹)	5.57×10^{-5}	1.76×10^{-5}	
v_l (ms ⁻¹)	3970	7956 (7141 ⁴²)	-
v_t (ms ⁻¹)	2670	4490 (4090 ⁴²)	-
v_m (ms ⁻¹)	2910	4990 (4544 ⁴²)	-
θ_D (K)	335	574 (522 ⁴² , 570 ⁴³)	-
B (GPa)	40.8	235 (185 ⁴² , 205 ³²)	-
γ	1.70	1.27	-

covalent bond in the a -axis direction, while by a weak van der Waals force in the c -axis direction.³⁹⁾ As shown in Fig. 1, SnO has a layered structure in the c -axis direction, while SnO₂ does not have such structure.

To check the validity of the values of α_L and α_V , we evaluated the parameters by direct measurements using a dilatometer (TD5000SA, Bruker AXS Inc.) under an Ar atmosphere. The temperature range was set as 300–673 K for SnO and 300–973 K for SnO₂. In the dilatometer measurement, the α_L can be defined by the following equation:

$$\alpha_L = \frac{1}{L_0} \frac{\Delta L}{\Delta T}, \quad (5)$$

where L_0 is the initial length, ΔL is the change of the length, and ΔT is the change of the temperature. The α_V can be calculated using the following relationship:

$$\alpha_V = 3\alpha_L, \quad (6)$$

Figure 9 shows the results of the dilatometer measurement. It can be confirmed that SnO shows larger thermal expansion than SnO₂. The α_L and α_V determined by the dilatometer measurements are summarized in Table 2. The α_V of SnO and SnO₂ are $5.57 \times 10^{-5} \text{ K}^{-1}$ and $1.76 \times 10^{-5} \text{ K}^{-1}$, respectively. These smaller values than those determined by the HT-XRD measurements would be caused by the effect of porosity. It has been suggested that the porosity suppressed the thermal expansion of bulk samples.⁴⁰⁾

In order to obtain accurate values of the sound velocity, the porosity correction was performed by using the measured sound velocities for three bulk samples of SnO with different porosity. The value corresponding to the sample with zero porosity was evaluated by linear extrapolation.⁴¹⁾ Since it was difficult to prepare several samples of SnO₂ with different porosity, the porosity correction for SnO₂ was done by using the same parameter obtained for SnO. The values obtained by the porosity correction of the longitudinal speed of sound (v_l) and transverse speed of sound (v_t) are summarized in

Fig. 9 Linear thermal expansion of SnO and SnO₂, measured by using a dilatometer.

Table 2, together with the literature data of SnO₂.^{32,42,43)} The average speed of sound (v_m), Debye temperature (θ_D), and bulk modulus (B) were calculated using the following equations:^{44,45)}

$$v_m^{-3} = \frac{(v_l^{-3} + 2v_t^{-3})}{3}, \quad (7)$$

$$B = d_0 \left(v_l^2 - \frac{4}{3} v_t^2 \right), \quad (8)$$

$$\theta_D = v_m \left(\frac{h}{k_B} \right) \left(\frac{3nN_A d_0}{4\pi M_W} \right)^{\frac{1}{3}}, \quad (9)$$

where d_0 is the theoretical density, h is the Planck constant, k_B is the Boltzmann constant, n is the number of atoms in the molecule, N_A is the Avogadro constant, and M_W is the molecular weight. The calculated values of the v_m , B , and θ_D of SnO are summarized in Table 2, together with the

literature data for SnO₂. It was confirmed that v_m , B , and θ_D of SnO are smaller than those of SnO₂.

The Grüneisen parameter (γ) which is related to the anharmonicity can be calculated as follows:⁴⁶⁾

$$\gamma = \frac{\alpha_V B V_M}{C_V}, \quad (10)$$

where V_M is the molar volume, C_V is the specific heat at constant volume which can be estimated by using Dulong-Petit law ($C_V = 3nR$ where R is the gas constant), and α_V is the volumetric thermal expansion coefficient evaluated by the HT-XRD method. Lattice anharmonicity is closely related with α_V , viz., large α_V means large anharmonicity. Therefore, the Grüneisen parameter (γ) can provide an indication of degree of anharmonicity as γ is proportional to α_V according to eq. (10). As summarized in Table 2, the calculated γ values were 1.70 for SnO and 1.27 for SnO₂. SnO with lone pair electrons clearly exhibits high γ value than SnO₂ with no lone pair electrons.

In order to find which parameter contributes to the difference in the κ_{lat} of SnO and SnO₂, we analyzed the κ_{lat} based on the following equation:⁴⁷⁾

$$\kappa_{\text{lat}} = A \frac{M \delta \theta_D^3}{N^{2/3} \gamma^2} \frac{1}{T}, \quad (11)$$

where A is a constant independent of the material, M is the average molar mass per atom, δ^3 is the average volume per atom, N is the number of atoms in the unit cell. At high temperatures above θ_D where Umklapp phonon-phonon scattering is dominant, the κ_{lat} can be calculated by eq. (11). Furthermore, the Grüneisen parameter (γ) is related to the relaxation time for Umklapp phonon-phonon scattering (τ_U), i.e., τ_U is proportional to γ^{-2} .⁴⁸⁾ Figure 10 shows the ratios of the parameters (SnO/SnO₂) of individual contributions for determination of κ_{lat} , where the ratio below 1 means that the parameter contributes to the lower κ_{lat} of SnO than that of SnO₂. As can be seen in Fig. 10, the SnO/SnO₂ ratios for γ and θ_D are less than 1, meaning that these parameters are dominant contributors to lowering κ_{lat} of SnO. Since the ratio for θ_D is smaller than that for γ , it can be said that the θ_D is more predominant than γ to reduce the κ_{lat} of SnO.

Figure 11 shows the temperature dependences of (a) σ , (b) S , (c) power factor $S^2\sigma$, and (d) zT of the bulk sample of SnO (sample #2). As can be seen in Fig. 11, these parameters increase with increasing temperature. The S values are positive, indicating that the SnO sample is p -type. The maximum values of the power factor and zT are $3.76 \mu\text{Wm}^{-1}\text{K}^{-2}$ @ 523 K and 0.00141 @ 573 K, respectively. Very recently, Miller *et al.* reported the experimental results on the TE properties of polycrystalline SnO bulk samples.⁴⁹⁾ These data are summarized in Table 3, together with the data of our sample. The n_H of our sample ($2.8 \times 10^{18} \text{ cm}^{-3}$ at room temperature) is clearly larger than the reported value ($1.0 \times 10^{16} \text{ cm}^{-3}$ at room temperature). The difference in the n_H between our sample and the sample reported in Ref. 49 would be caused by the difference in the amount of impurities existed in the samples. Miller *et al.* synthesized the SnO powders through a precipitation reaction method using SnCl₂ as a precursor, where high-

Fig. 10 Ratios of the parameters (SnO/SnO₂) of individual contributions for determination of κ_{lat} .

Table 3 Results of the Hall effect measurements and the Seebeck coefficient of the bulk sample of SnO (sample #2). The literature data for SnO⁴⁹ are shown for comparison. All the data are obtained at room temperature.

	ρ	Carrier	n_H	μ_H	S
	(Ωcm)	type	(cm^{-3})	($\text{cm}^2\text{V}^{-1}\text{s}^{-1}$)	(μVK^{-1})
SnO	7.36	p	2.8×10^{18}	0.30	371
SnO ⁴⁹	40	p	1.0×10^{16}	30	635

purity SnO powders compared with the commercial grade could be obtained. Here, we used commercially-available SnO powders (99.9%), and impurities existed in the powders would act as hole dopants and increase the n_H . Due to this large n_H , our sample shows small S and low μ_H compared with those reported in the literature. We will try to enhance the TE properties of SnO through the carrier concentration optimization. The results will be reported in near future.

4. Conclusion

It is considered that SnO can be a good TE material because it has lone pair electrons and thereby has large anharmonicity and low κ_{lat} . However, a fine bulk sample of SnO has been never synthesized because SnO is easily decomposed into SnO₂ and Sn even at 700 K. In the present study, we succeeded in synthesizing high-density pure bulk SnO samples by using high-pressure and low-temperature SPS (500 MPa, 598 K). It was revealed that SnO has much smaller κ_{lat} values ($1.44 \text{ Wm}^{-1}\text{K}^{-1}$ at 573 K) than SnO₂ which has no lone pair electrons. It was confirmed that not only large Grüneisen parameter ($\gamma = 1.70$) but also low Debye temperature ($\theta_D = 335 \text{ K}$) contributes to this low κ_{lat} of SnO. Furthermore, we reported the TE properties of SnO, where the maximum values of the power factor and

Fig. 11 Temperature dependences of (a) electrical conductivity σ , (b) Seebeck coefficient S , (c) power factor $S^2\sigma$, and (d) dimensionless figure of merit zT of the bulk sample of SnO (sample #2).

zT are $3.76 \mu\text{Wm}^{-1}\text{K}^{-2}$ @ 523 K and 0.00141 @ 573 K, respectively. The TE properties can be enhanced through the carrier concentration optimization.

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