## The highest thermoelectric figure of merit biology essay

Science, Biology



## ABSTRACT

The highest thermoelectric figure of merit ZT = 1. 33 is achieved at 650 K in the sample p-type Ag(Sb1-xlnx)Te2 with x = 0.03, representing a more than 50% enhancement with respect to an undoped AgSbTe2. This enhancement of ZT can be mainly attributed to a remarkable decrease in lattice thermal conductivity due to enhanced phonon scattering mechanism and great enhancement in power factor due to increase in electrical conductivity by indium doping. This result shows promising thermoelectric properties in the medium temperature range. The rousing worldwide concern over our reliance on fossil fuels is driving the need for alternative energy sources and novel energy conversion techniques, among which the thermoelectric (TE) technique has several special features such as its all solid-state assembly without moving parts, comfort of switching between the power generation mode (based on the Seebeck effect) and the refrigeration mode (based on the Peltier effect), low cost maintenance and its capability to easily couple to other energy conversion devices. Thermoelectric effects associate with direct conversion between thermal and electrical energy by employing electrons and holes as energy carriers. Such effects are potentially useful for waste heat recovery and environmentally friendly refrigeration. 1, 2 The performance of TE devices is assessed by the dimensionless figure of merit (ZT), defined as  $ZT = \alpha 2\sigma T/\varkappa$ , where  $\alpha$ ,  $\sigma$ , T and  $\varkappa$  are the Seebeck coefficient, the electrical conductivity, the absolute temperature and the thermal conductivity, respectively. Since  $\alpha$ ,  $\sigma$ , and the electronic contribution to *\** are involve via band structures (energy gap Eg, effective mass carrier m<sup>\*</sup>, etc.) and scattering mechanisms, it is difficult to control the parameters https://assignbuster.com/the-highest-thermoelectric-figure-of-merit-biologyessay/

independently. 1 Therefore,  $ZT \not \sim 1$  has been considered as a benchmark for many thermoelectric materials for a long time. Based on the above relation, the best performance TE materials should have high electrical conductivity, large Seebeck coefficient and low thermal conductivity. 1AgSbTe2 has been known as a potential thermoelectric material for a long time3-11 due to its relatively low thermal conductivity (0.  $6 \sim 0.7$  Wm-1K-1). 12, 13 AgSbTe2 is widely identified as the disordered NaCl type (Fm-3m) where Ag and Sb randomly occupy the Na site. 14 According to the previous studies, 11 the disordered lattice structure dominantly contributes to low lattice thermal conductivity through Umklapp and intrinsic phonon-phonon scattering processes without significant reduction in the electrical conductivity. Recently, the AgSbTe2 compound has attracted much attention to construct the so called bulk nanostructured TE materials such as (AgSbTe2)1-x(PbTe)x(also called LAST) and (AgSbTe2)1-x(GeTe)x (also called TAGS) with excellent TE properties. 15-20Doping is a possible approach to optimize the thermoelectric properties of p-type AgSbTe2 by reducing its thermal conductivity and adjusting its carrier concentration. In this study, trivalent In3+ ions were selected to substitute Sb3+ ions in a p-type Ag(Sb1-xInx)Te2 systems in order to suppress lattice thermal conductivity dramatically while simultaneously contributing to the total charge-carrier concentration. Meanwhile, to the best of our knowledge, In-substitution in p-type AgSbTe2 has not been reported so far. Thus, the influence of In doping on the thermodynamic properties, microstructure and TE transport behavior in the Ag(Sb1-xInx)Te2 compounds was systematically investigated in this study. Polycrystalline Ag(Sb1-xInx)Te2 compounds with x = 0, 0.03 and 0.05 were

prepared by solid state reaction. High-purity starting elements of Ag (99. 995%, filament), Sb (99. 9999%, shot), In (99. 999%, shot) and Te (99. 999%, shot), were melted in carbon coated guartz tubes with diameter of 1. 6 cm under the vacuum at 800 °C for 6 h, then slowly cooled to 475 °C, followed by a rapid guenched in water. The obtained ingots were pulverized to powder, the mixed powder then sealed in guartz tubes under a vacuum of about 10-4 Torr after multiple argon gas purging cycles, pretreated at 500 °C for 18 h in a box furnace, and furnace cooled to room temperature. Single crystals were grown with a vertical Bridgman furnace starting from the pretreated powder and vacuum sealed in carbon coated guartz tubes of 10 cm length and 1. 6 cm in diameter, the temperature profile of the Bridgman furnace used for the whole series was maintained at 450-700 °C within 25 cm region. Initial complete melting was achieved at 700 °C for 24 h to ensure complete reaction, mixing and cooled (1 °C h-1) to 500 °C, then annealed for 48 h and the guartz tube was then slowly lowered into the cooling zone at a rate of  $\sim 0.5$  mmh-1. Highly dense ingots with dark silvery metallic shine were obtained. These ingots which were stable in water and air were then cut and polished into rectangular shapes of approximately 3x3x12 mm3, and circular discs of diameter 12 mm and thickness 1 / 2 mm for later physical properties measurements. The density of the ingots measured by the Archimedes method varied from 7. 11~7. 12 gcm-3 which is  $\sim$  99.9% of the theoretical density. X-ray diffraction experiments were conducted for phase identifications using a powder X-ray diffractometer (X'Pert PRO-PANalytical, CuK $\alpha$  radiation) at 2 $\circ$  angles of 20-80°. With these data, lattice parameters of Ag(Sb1-xlnx)Te2 (x = 0, 0.03 and 0.05) samples

were calculated by the Rietveld refinement program. Fractured surface morphology was characterized with a field emission scanning electron microscopy (FESEM, Hitachi, S-4800). The chemical composition of the asprepared ingots was determined by wavelength dispersive X-ray fluorescence spectrometry (WD-XRF). The Hall Effect was measured at room temperature under 0.55 T with a four probe configuration using the van der Pauw method (ECOPIA HMS-5000). The electrical conductivity  $\sigma$  and Seebeck coefficient  $\alpha$  were measured simultaneously by a commercial equipment (ZEM-3, ULVAC-RIKO, Japan) in He atmosphere from 300 to 700 K. Thermal conductivity  $\kappa$  was calculated using the equation  $\kappa = DCpd$  from the thermal diffusivity D obtained by a laser flash apparatus (NETZSCH, LFA 457), specific heat Cp determined by a differential scanning calorimeter (NETZSCH, STA 449), and the density d obtained by the Archimedes method. FIG. 1. (Color online) (a) Powder XRD patterns of Ag(Sb1-xInx)Te2 samples and (b) SEM photographs of the bulk Ag(Sb0. 97In0. 03)Te2. The inset of (b) shows its magnified portion. The samples of Ag(Sb1-xInx)Te2 were obtained as crystalline ingots, they were then cut and polished for the transport property measurements presented here. Fig. 1(a) represents powder X-ray diffraction (XRD) patterns of samples with composition Ag(Sb1-xInx)Te2 (x = 0, 0. 03, and 0. 05). It is clear that in addition to the main phase of AgSbTe2 solid solution (space group Fm-3m, reference code: 01-089-3671) in all the samples, small amount of Sb2Te phase (marked with the arrow, reference code: 01-080-1722) is detected in the samples with x = 0.03 and x = 0.05. As shown in the inset of Fig. 1(a) indicates that the relative intensity of Sb2Te peak increases with increasing the content of In and also the

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characteristic peaks of the AgSbTe2 phase shift to lower 20 angles with increasing x, indicating that the lattice parameter increases with the increasing In content. According to our Rietveld refinement, the lattice parameters are 6. 078(0) Å (1 Å = 0. 1 nm), 6. 0842(1) Å, and 6. 0844(0) Å for x = 0, 0.03 and 0.05, respectively. This nearly linear increase of the lattice parameter with the increasing In content is expected, since the radius of  $In3+ (\square 0.81 \text{ Å})$  is larger than that of Sb3+ ( $\square 0.76 \text{ Å}$ ), which implies that In3+ indeed replaces Sb3+ in the crystal lattice. Fig. 1(b) shows the FESEM photograph of the fracture free surface of the Ag(Sb0. 97In0. 03)Te2 sample. The magnified photo (the inset of Fig. 1b) shows that nanoprecipitate rich in Sb2Te with a feature size of few hundred nanometers are distributed at grain boundaries. TABLE I. Carrier concentration n, Hall mobility µH, electrical conductivity  $\sigma$ , Seebeck coefficient  $\alpha$  and measured composition of all samples at room temperature. Nominal compositionMeasured compositionn ( 1019cm-3)μH(cm2V-1s-1)σ104 (Sm-1)α (μVK-1)AgSbTe2Ag0. 96Sb1. 05Te24. 527. 622229Ag(Sb0. 97 In0. 03)Te2Ag(Sb0. 98 In0. 023)Te28. 722. 643. 17193Ag(Sb0. 95 In0. 05)Te2Ag(Sb0. 92 In0. 046)Te26. 322. 152. 6211. 7The average compositions of the AgInxSb1-xTe2 series obtained from wavelength dispersive X-ray fluorescence analysis were closely consistent with the nominal compositions (Table I). Fig. 2 shows the temperature dependences of the charge transport properties of Ag(Sb0. 97In0. 03)Te2 samples. As expected, the sample with higher electrical conductivity has a lower Seebeck coefficient, and the trend of  $\alpha$  versus T curve is basically reflected from that of the  $\sigma$  versus T curve in Figs. 2(a) and 2(b), respectively. The temperature dependence of the electrical conductivity for

Ag(Sb1-xInx)Te2 series decreases with increasing temperature, after which the electrical conductivity increases with increasing temperature. Moreover, as In content x increases from 0 to 0. 03, electrical conductivity of Ag(Sb1xInx)Te2 increases remarkably, however with further increase in x electrical conductivity decreases due to decrease in carrier concentration. The sample with x = 0.03 has the highest electrical conductivity among all the samples with a value of about 3. 17 x 104 Sm-1 at 300 K. Table I shows the properties used to describe the electron transport characteristics of In doped Ag(InxSb1-x)Te2 compounds at room temperature. Compared with undoped sample, the In-AST samples display high carrier concentration and lower mobility. The Seebeck coefficients of all the specimens are positive, as shown in Fig. 2(b), indicating the p-type conduction. At room temperature, the Seebeck coefficients ( $\alpha$ ) for In-AST samples span from 190 to 215  $\mu$ VK-1, slightly lower than that of the undoped AgSbTe2 sample. The increased electrical conductivity and the decreased Seebeck coefficient of the sample with x = 0.03 can be ascribed to the increased carrier concentration due to the In-doping effect, which is similar to that in the Se-doped AgSbTe2 sample. 11 The power factor P. F. =  $\alpha 2$ ?, curves are plotted in Fig. 2(c), the power factor initially increases, reaches maximum and then decreases with increasing temperature. The sample with x = 0.03 has the highest power factor P. F. among the three samples with a peak P. F. value  $\sim 1.42 \approx 10-3$ Wm-1K-2 at 540 K. Fig. 2(d) shows the temperature dependence of the total thermal conductivity of the Ag(Sb1-xInx)Te2 samples. FIG. 2. (Color online) Temperature dependences of (a) electrical conductivity, (b) Seebeck coefficient and (c) power factor for samples of Ag(Sb1-xlnx)Te2 (x = 0, 0.03,

and 0. 05). Fig. 3(a) shows the temperature dependence of thermal diffusivity D and measured specific heat capacity Cp of Ag(Sb1-xInx)Te2 samples. From the specific heat data, the results closely matches the literature value (Cp  $\sim$  0. 205 Jg-1K-1) of AgSbTe2. 12 Total thermal conductivity is calculated as a product of the measured specific heat at constant pressure Cp, thermal diffusivity D and material density d. Fig. 3(b) shows the temperature dependence of the total thermal conductivity of the AgInxSb1-xTe2 samples. For all samples the # first decreases and then increases with increasing temperature and the magnitude spans from 0.65 to 0.9 Wm-1K-1. The thermal conductivity of the sample with x = 0.03exhibits lowest thermal conductivity than all other samples over the temperature range from 300 to 700 K with the minimum × 0. 66 Wm-1K-1 at 570 K. In general, In-AST samples show lower thermal conductivities than that of undoped AgSbTe2 sample. Near room temperature, bulk of the heat is conducted by long-wavelength acoustic phonons3 and the rapid increase in thermal conductivity at high temperatures may be related to an enhancement in ambipolar thermal conductivity. 21 Using the Wiedmann-Franz law,  $\varkappa e = L\sigma T$ , where L is the Lorentz constant, the lattice thermal conductivity **\***L can be estimated by subtracting the electronic thermal conductivity  $\varkappa$  e from the total thermal conductivity  $\varkappa$ ,  $\varkappa$  L =  $\varkappa$  - LoT. For a degenerate semiconductor L = 0. 7L0 (L0 =  $\pi 2/3$ (kB/e)2 = 2. 45x10-8 V2K-2). 21 As shown in Fig. 3 (c), the **\***L of In-AST samples increases with increasing In substitution fraction. The sample with x = 0.03 exhibits lowest lattice thermal conductivity (~ 0. 42 Wm-1K-1) than undoped AgSbTe2 (~ 0. 59 Wm-1K-1) at 650 K, closing to the minimum theoretical thermal

conductivity (~ 0. 3 Wm-1K-1) calculated from formulas reported by Cahill et al. 22 The reason for the very low lattice thermal conductivity in Ag(Sb0. 97In0. 03)Te2 may be the nanoprecipitates rich in Sb2Te with a feature size of few hundred nanometers as shown in Fig. 1(b) that are effective in scattering the phonons with mid-to-long mean free paths 23. FIG. 3. (Color online) Temperature dependences of (a) Diffusivity and specific heat, (b) total thermal conductivity and (c) lattice thermal conductivity of Ag(Sb1 $x \ln x$ )Te2 (x = 0, 0. 03, and 0. 05). The dimensionless thermoelectric figure of merit ZT is calculated from the measured values of  $\sigma$ ,  $\alpha$ , and  $\varkappa$  using the equation  $ZT = \alpha 2\sigma T/\varkappa$ . Fig. 4 shows the temperature dependence of ZT of all Ag(Sb1-xInx)Te2 (x = 0, 0.03 and 0.05) compounds. While at room temperatures the values of ZT of all samples are comparable, at elevated temperatures the benefit of In doping is more clearly demonstrated. The highest figure of merit is observed in Ag(Sb0. 97In0. 03)Te2, it reaches 1. 33 at 650 K because of the relative higher power factor and lower thermal conductivity among all samples. This value is 50% higher than that of the undoped AgSbTe2 at the same temperature. FIG. 4. (Color online) Temperature dependences of thermoelectric figure of merit ZT for samples of Ag(Sb1-xlnx)Te2 (x = 0, 0.03, and 0.05). In summary, the TE properties of In-doped Ag(Sb1-xInx)Te2 compounds have been investigated. XRD analysis indicates that single phase material crystallizing in a cubic NaCltype structure in In-doped AgSbTe2 samples. The lattice thermal conductivities were greatly reduced by enhanced phonon scattering, and the power factors were enhanced due to increase in electrical conductivity compared to undoped sample. The best TE performance is achieved for the

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sample with x = 0.03, since the substitution of In for Sb leads to the increased carrier concentration and the enhanced phonon scattering. A maximum ZT value of 1. 33 is obtained at 650 K for the sample with x = 0. 03, this value is 50% higher than that of the undoped AgSbTe2 at the same temperature. These results indicate that slight doping with In on Sb site is an effective way to enhance the thermoelectric performance of p-type AgSbTe2. This work was supported by Academia Sinica and National Science Council, Taiwan, Republic of China, under Grant No. NSC100-2112-M-001-019-MY3.