



Realized high power factor and thermoelectric performance in Cu_2SnSe_3

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ABSTRACT

New thermoelectric compounds $\text{Cu}_2\text{Sn}_{1-x}\text{Fe}_x\text{Se}_3$ ($0 \leq x \leq 0.2$) have been investigated, and the results indicate that the electrical conductivity of $\text{Cu}_2\text{Sn}_{1-x}\text{Fe}_x\text{Se}_3$ ($x > 0$) is obviously enhanced by Fe doping due to the increased carriers concentration, and then the significant improved power factor is obtained. As a result, the figure of merit reaches 1.1 at ~ 820 K for Fe-doped compounds $\text{Cu}_2\text{Sn}_{1-x}\text{Fe}_x\text{Se}_3$ with $x = 0.05$ and 0.1 due to the higher power factor and moderate thermal conductivity, which is about 2.4 times that of pure Cu_2SnSe_3 at the same temperature. Our results indicate that Fe-doped compounds $\text{Cu}_2\text{Sn}_{1-x}\text{Fe}_x\text{Se}_3$ can be hoped to utilize as a potential environmental thermoelectric materials.

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Thermoelectrics can transfer energy from heat to electricity or vice versa without any pollution and moving parts [1], and thus it attracts more and more interesting research due to its environmental character. Generally, the conversion efficiency of thermoelectric materials is mainly characterized by the figure of merit $ZT = S^2 \sigma T / \kappa$, where S is the Seebeck coefficient, σ is electrical conductivity, T is absolute temperature and κ is thermal conductivity, respectively. In order to improve thermoelectric performance, many researches have been executed to focus on some material systems [2–4], PbTe , Bi_2Te_3 and so on. PbTe and Bi_2Te_3 system based materials present the good thermoelectric application in the middle temperature range and near room temperature, respectively. As an environmental friendly method to recover waste heat, its application should be limited because of the existence of toxic or harmful elements in both PbTe and Bi_2Te_3 . Thus, recently, some environmental friendly materials have absorbed many research interests, such as Cu_2SnSe_3 [5], Cu_3SbSe_4 [6], SnSe [7], $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ [8], without Pb and/or Te.

Cu_2SnSe_3 belongs to face centered cubic structure with space group $F\bar{4}3m$ (216) at room temperature. Cu and Sn share the same atomic positions 4a site (0, 0, 0) with an occupancy of 0.67 and 0.33, respectively, while full occupancy of Se at the 4c site (0.25, 0.25, 0.25). Cu_2SnSe_3 is usually investigated as a likely candidate for photo-voltaic and acousto-optic applications [9]. Recently, Cu_2SnSe_3 has been reported as a potential thermoelectric material with really good performance [5,10,11].

Here, we present a primary research on the thermoelectric properties of Cu_2SnSe_3 by Fe doping. The results indicate that higher power

factor and ZT values are obtained after Fe doping, especially, ZT value reaches 1.1 for $\text{Cu}_2\text{Sn}_{0.95}\text{Fe}_{0.05}\text{Se}_3$ and $\text{Cu}_2\text{Sn}_{0.9}\text{Fe}_{0.1}\text{Se}_3$, which is about 2.4 times that of pure Cu_2SnSe_3 at the same temperature ~ 820 K. Our research supplies a new method to develop the thermoelectric performance of Cu_2SnSe_3 .

Polycrystal $\text{Cu}_2\text{Sn}_{1-x}\text{Fe}_x\text{Se}_3$ ($x = 0, 0.05, 0.1, 0.15$ and 0.2) was prepared by a fusion method. Elemental copper (3N), tin (5N), iron (AR.) and selenium (5N) powders (Alfa Aesar) were weighed accurately according to the desired composition, and sealed in an evacuated quartz tube, which were heat-treated in horizontal furnace at 1193 K for 8 h with the heating rate of 5 K/min, and then furnace cooled to 973 K soaked 48 h, finally, cooled to room temperature. The obtained ingot was ground into powders. The powders of about 2.5 g were compacted by hot-pressing technique at a pressure of 250 MPa and 673 K in a diameter of ~ 15 mm tungsten carbide die in vacuum for 1 h with heating rate of 7 K/min, respectively. After a natural cooling process, bulk sample with dimensions of cylinder $\Phi 15$ mm \times ~ 2 mm in thickness was obtained.

The product was characterized by X-ray diffraction (XRD) using Philips X'Pert PRO X-ray diffractometer equipped with graphite monochromatic Cu-K α radiation ($\lambda = 1.54056$ Å). The microstructure was characterized by field emission scanning electron microscopy (FESEM; SU8020). The density D of hot-pressed bulk samples was determined by the Archimedes' method. The electrical conductivity σ and the Seebeck coefficient S were measured by using a commercially available instrument (ULVAC, ZEM-3) in He atmosphere. Thermal diffusivity (α) was measured by the laser flash method using a Netzsch LFA 457 instrument. The heat capacity C_p was obtained with a differential scanning calorimeter (DSC) (Perkin-Elmer, USA). Thermal conductivity κ was calculated based on the relationship $\kappa = \alpha \cdot C_p \cdot D$. Our samples present the higher stability in the investigated temperature range; indeed, there

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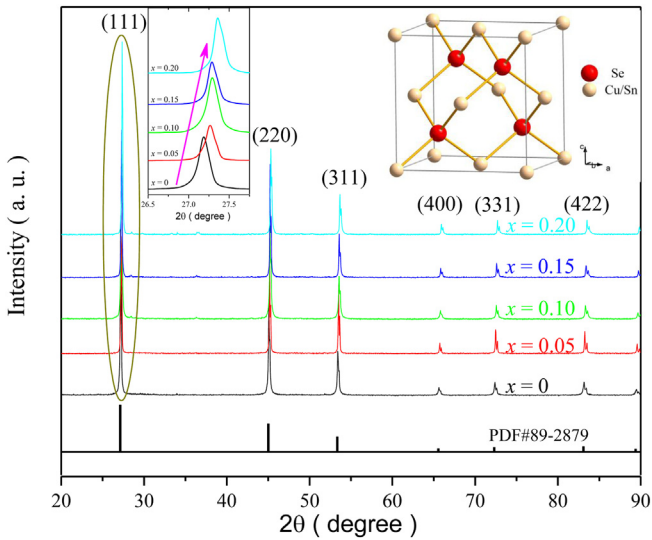


Fig. 1. Powder XRD patterns of polycrystalline samples $\text{Cu}_2\text{Sn}_{1-x}\text{Fe}_x\text{Se}_3$ ($x = 0, 0.05, 0.1, 0.15$ and 0.2); left insert is enlarged (111) peaks for all samples; right insert presents the crystallographic structure of Cu_2SnSe_3 .

Table 1

The refined lattice parameter a from XRD patterns, fitted hole concentration p , hole mobility μ and the relative density for Fe-doped compounds $\text{Cu}_2\text{Sn}_{1-x}\text{Fe}_x\text{Se}_3$ ($x = 0, 0.05, 0.1, 0.15$ and 0.2).

x	a (10^{-10} m)	p (10^{26} m^{-3})	μ ($\text{cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$)	Relative density (%)
0	5.7007	1.91	14.3	98.4
0.05	5.6894	2.99	28.2	98.1
0.1	5.6859	3.49	39.4	98.6
0.15	5.6807	5.63	37.7	98.4
0.2	5.6811	5.31	29.6	98.8

almost have no changes for the sample after measurement. The density of states is calculated by using Cambridge Serial Total Energy Package (CASTEP) software. The exchange correlation functional is selected as the generalized gradient approximation of Perdew–Burke–Ernzerhof (GGA-PBE) [12].

Fig. 1 shows the powder XRD patterns of polycrystalline samples. It can be seen from Fig. 1 that the main diffraction peaks for all samples can be indexed to the phase of Cu_2SnSe_3 (PDF#89-2879), belonging to the face center cubic structure, indicating that the specimens have the same crystallographic structure as that of Cu_2SnSe_3 (right insert of Fig. 1). It is noticeable that the peaks for the Fe-doped samples slightly shift to high angle. As shown in the left insert of Fig. 1, the enlarged (111) peaks for all specimens, we can clearly find that (111) peak shifts to high angle with increasing the Fe content, which may result from the shrink of crystal lattice after Fe doping. In order to examine the variation of crystal lattice, Rietveld refinements have been performed on the XRD results, which generate the values of lattice parameter a , as shown in Table 1. We can see from Table 1 that the lattice parameter a decreases with increasing the Fe content, which is consistent with the change of diffraction peaks in the XRD patterns. Indeed, the ionic radius of Fe^{3+} (0.63 Å) is slightly smaller than that of Sn^{4+} (0.69 Å), the crystal lattice should shrink after the substitution of Sn^{4+} by Fe^{3+} . However, when Fe content x exceeds 0.15 and reaches 0.2, the lattice parameter a increases slightly, which may mean the solution limit of Fe in the $\text{Cu}_2\text{Sn}_{1-x}\text{Fe}_x\text{Se}_3$ is between in this range.

Fig. 2 shows the images of scanning electron microscopy (SEM) and results of energy dispersive spectrometer (EDS) for pure Cu_2SnSe_3 and Fe doped specimen with $x = 0.1$. We can see from Fig. 2(a) and (b) the size of grains distributed from several hundred nanometers to several micrometers and does not obviously change after Fe doping. Fig. 2(d–h) presents the EDS mapping results on the area of Fig. 2(c), which shows that all the elements (Cu, Sn, Fe, Se) exist and evenly distributed in the crystalline.

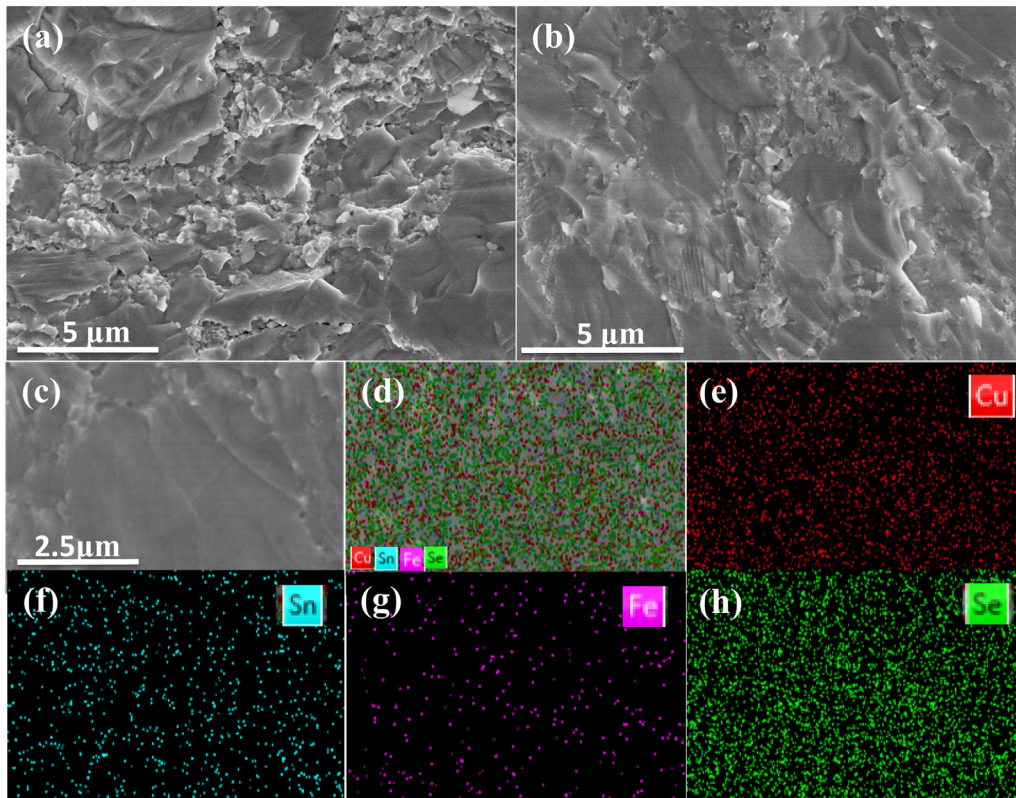


Fig. 2. SEM images of Cu_2SnSe_3 (a) and $\text{Cu}_2\text{Sn}_{0.9}\text{Fe}_{0.1}\text{Se}_3$ (b, c), (d)–(h) are the EDS results in the (c) area for total elements, Cu, Sn, Fe and Se, respectively.

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