Thermoelectric Properties of C₆₀ Doped Bi_{0.5}Sb_{1.5}Te₃

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Abstract

This work includes thermoelectric $Bi_{0.5}Sb_{1.5}Te_3$ compounds doped with C_{60} . Synthesis of thermoelectric materials includes elemental shots of Bismuth (Bi), Antimony (Sb), and Telluride (Te). An allotrope of Carbon, fullerene, was doped into the materials and thermoelectric properties of the materials is investigated. Fullerene molecules reduce the lattice thermal conductivity in the sample is studied for enhancing the dimensionless thermoelectric figure of merit (ZT). The fabricated samples are measured in the temperature range of 50°C to 255°C

Introduction

Thermoelectricity is the conversion of heat into electricity. Thermoelectric materials describes materials that effectively converts heat into electricity.¹ Some applications are thermoelectric generators, thermoelectric cooling, and thermocouples. Thermoelectric generators assist in energy recycling in power plants and increased fuel efficiency of automobiles. Thermoelectric cooling is found in refrigeration systems to maintain specific temperatures. Thermocouples measure the temperature differences between two objects. The focus of the study is view thermoelectric materials with the addition of fullerene molecules. Thermoelectric materials have high potential in conversion of waste heat and thermal energies into electrical energy.² Thermoelectrics may attribute to the growth of renewable energy applications and allows consumers to reduce dependence on fossil fuels. Thermoelectric technology itself has no vibration, quiet, and no moving parts. Thus, efficiency of thermoelectrics is significantly important for various applications. The efficiency is measured by the dimensionless thermoelectric figure of merit³ as,

2

$$ZT = \frac{S^2T}{\rho k}$$

where *S* is the Seebeck thermoelectric coefficient; *T* is the temperature; *k* is the thermal conductivity; and ρ is the electrical sensitivity. ZT improvement is the focus of the research and with high ZT>1⁴, applications of thermoelectric materials can become vast. Reducing thermal conductivity allows ZT improvement and with the introduction of C₆₀ fullerene to the thermoelectric materials the electrical conductivity is enhanced. The electrical conductivity is significantly important and evaluates how strong the sample will conduct an electric current.

Method

The samples were obtained through fabrication by mechanical methods. Elemental shots were placed through ball milling, cold pressing and heat treatments. A molar ratio of Bi, Sb, and Te respectively of 3, 6 and 9 were placed in a sealed vial and allowed to ball mill for forty hours in a glove box [Figure 1], by PLAS LABS, under argon gas.



Figure 1.

Reducing oxygen and outside environmental air exposure as much as possible, if not completely. With the reduction of oxidation the attribute of the samples will high resistance to creeping, or crack and deforming under stresses, at high temperatures, high strength, and corrosion resistance.⁵ The reduction is critical in obtaining an appropriate sample. After the sample has successfully ball milled; it is now separated and allowed introduction of C_{60} fullerene. Concentrations of 0.35% and 0.5% wt are now applied into the ball milled samples. A sample of pure $Bi_{0.5}Sb_{1.5}Te_3$ is needed to ensure accuracy of ZT measurement. All three samples are placed in a clay tubes and allowed to *bake* in a SentroTech high temperature furnace. [Figure 2]



Figure 2.

A temperature curve of temperature in Celsius and time must be apportioned for ten hours for the sample powders' accurate fabrication. The sample powders will be undergoing temperatures upwards of 400°C within the ten hours in the furnace. Within the furnace the sample powders will be fabricated in a hydrogen rich environment. The heat treatments can allow cracking of the sample if temperature is not accurately apportioned.⁶ The appropriate temperature time consists of a heating rate at 2°C/min and multi-step annealing was used: at 280°C for two hours, 340°C for two hours, 380°C for five hours, and allowed to cool for one hour. Specifically, sample was left overnight to cool. [Figure 3]



Finally the sample powders are cold pressed with dies into disks with the thickness of the pure $Bi_{0.5}Sb_{1.5}Te_3$ (3.70mm), $Bi_{0.5}Sb_{1.5}Te_3$ -C₆₀0.35% (3.94mm), and $Bi_{0.5}Sb_{1.5}Te_3$ -C₆₀0.5% (3.90mm). The disks are collected and cut into ingots and placed in a Seebeck Coefficient/

Electric Resistance Measuring device, or a ZEM-3 instrument, by ULVAC. [Figure 4]



Figure 4.

The instrument simultaneously measures the electrical resistivity and Seebeck coefficient of the fabricated alloys. The samples are measured in the temperature range of 50°C to 255°C.



Figure 5.

Figure 5 shows the sample after cold pressing. The final fabrication required the sample power to be placed in the dies and allowed to compress for one hour before removal. Final sample results in the disk-shaped alloy.

Results and Discussion

The dimensionless thermoelectric figure of merit obtained from the ZEM-3 machine measured samples highly dependent on the temperature and the concentration of C_{60} doping. Figure 6(b) shows the figure of merit to be between 0.89 and 1.01 in the temperature range of 75°C to 150°C. This sample shows better thermoelectric performance for applications for this temperature range; whereas, Figures 6(a) and 6(c) share a lower thermoelectric figure of merit, respectively.





The fullerene free sample, pure, has significantly less ZT than the sample with the concentration of 0.35% C_{60} doping. This enhancing is understood to be the reduction of lattice thermal conductivity. The objective is to reach ZT>1, which is achieved, and is ideal in an atomic scale. Figure 6(b) is arguably relatively close to the ideal ZT value. The temperature dependence limits the application that may be used for the devices and with the ZT values varying between 6(a) and 6(c) the applications of doping C_{60} is also limited. The result of 6(b) being the ideal ZT value shows that it is quite possible that the higher concentration of C_{60} limits the conductivity of electricity; since 6(c) and the ZT value is much lower than 6(a). Figure 7 gives a simple understanding of ZT efficiency.



Figure 7

Conclusion

This work was a success in fabrication and study of $Bi_{0.5}Sb_{1.5}Te_3$ with C_{60} . Bismuth telluride based alloys are some of the highest thermoelectric performance materials, which are used for waste heat harvest. However, these materials still operate at a relatively low efficiency. With the introduction of C_{60} fullerene molecules to the material structure; the thermoelectric figure of merit of the material is increased significantly. The C_{60} concentration of 0.35wt% warrants promising results for thermoelectric applications. Specifically, in the temperature range of 75°C to 150°C, good thermoelectric figure of merit of the sample is between 0.8 and 1.0. The addition of C_{60} reduced the lattice heat conductivity and is an enhancement of the figure of merit. Certainly ZT efficiency may increase with ongoing effort by researchers and leading to a material that produces a significant role for a more attractive renewable energy source. Recovery of waste heat is highly valuable in renewable resource and with better ZT efficiency recovery will be achieved.

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