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Grain size mediated electrical and thermoelectric performances of mechanically alloyed Sb_2Te_3 nanoparticles

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ABSTRACT

Antimony telluride (Sb_2Te_3) nanoparticles of different sizes were fabricated by mechanical alloying (MA) of elemental Sb and Te powers for different durations. The powder nanostructures were pelletized, annealed in Ar ambient, and characterized by XRD, FESEM, TEM to study the effect of milling time and thermal treatment on particle size, grain growth, and crystallinity. The annealed and unannealed pelletized nanostructures were analyzed in a PPMS to study the effect of grain growth on their electrical and thermoelectric properties. Room temperature electrical conductivity of the p-type semiconductor nanostructures improved significantly (from ~10^3 to ~ 10^5 mho/m) due to thermal annealing and results in the considerable improvement in thermoelectric figure of merit (ZT). Thermal annealing-induced grain growth also transforms the semiconducting nature of the sample to metallic. The reduced thermal conductivity of the nanostructures with reduced grain size improves the ZT. The temperature-dependent Lorenz number ($L_{effective}$) is used to find the electronic contribution of total thermal conductivity, and it is explained by the non-parabolic Kane model.

1. Introduction

Thermoelectric materials are efficient converters of waste heat into useable electrical energy due to their high Seebeck coefficients [1,2]. Thermoelectric figure of merit ZT defines the performance of a thermoelectric material in converting thermal energy to electricity. The ZT is defined as, $ZT = S^2\sigma T/K$, where S,σ, and K represent the Seebeck coefficient, electrical conductivity, the thermal conductivity of the material, respectively, and T is the temperature in K [3]. The $S^2\sigma$ term is defined as the power factor. Owing to the demand for alternative energy sources, the quest for new materials with an improved figure of merit (ZT) has increased globally at a rapid rate [4,5].

In general, semiconductors are better thermoelectric materials compared to metals [6]. According to Wiedemann-Franz law [7], most metals have a nearly constant electrical to thermal conductivity ratio, and increasing electrical conductivity is difficult without increasing their thermal conductivity. However, a good ZT value requires a high electrical conductivity and simultaneously a lower thermal conductivity. Hence, for metals or metallic alloys, the only possible way to obtain a significant figure of merit is to have a high value of the Seebeck coefficient. Unfortunately, most metals show very small Seebeck coefficients (~10 μV/K), and their thermoelectric efficiencies are only fractions of a percent. On the other hand, semiconductors with comparatively higher Seebeck coefficient values (~100 μV/K) had drawn strong attention as thermoelectric materials since 1920 [8]. Low bandgap semiconductors possess high electrical conductivity, comparable to metals. Compared to bulk materials, nanomaterials have low thermal conductivity because of lower lattice thermal conductivity resulting from the increased phonon scattering due to smaller grain size [9–12]. Thus, nanostructured semiconductors of smaller bandgaps are considered the most favorable thermoelectric materials as they produce a reasonably higher figure of merit values.

Antimony telluride (Sb_2Te_3), a low bandgap semiconductor, has been considered as one of the promising thermoelectric materials for low-temperature applications [13–15]. Nano-structured Sb_2Te_3 thin films fabricated by physical vapor deposition [16], metal-organic chemical vapor deposition [17,18], thermal co-evaporation [19], flash evaporation [20], electrochemical method [21], ion beam sputtering [22], molecular beam epitaxy [23] etc. have shown good thermoelectric conversion efficiency. On the other hand, single-phase Sb_2Te_3 nanoparticles synthesized by microwave-assisted

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Improved thermoelectric performance of nanostructured Bi_2Te_3 fabricated by solvent-free mechanical alloying

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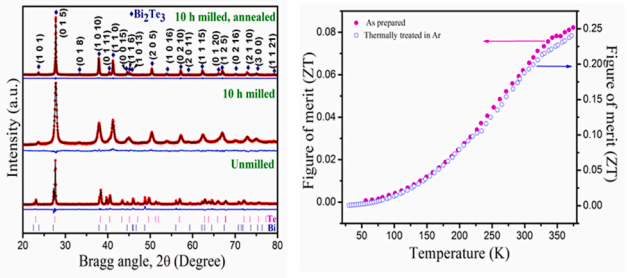
HIGHLIGHTS

- Nanostructured Bi_2Te_3 has been synthesized by facile mechanical alloying method.
- Microstructures of the samples are characterized by XRD and FESEM.
- The semiconducting nature of the sample changes to metallic after annealing.
- Grain growth and associated band gap reduction is noticed after annealing at 573K.
- About three times increase in thermoelectric figure of merit owing to annealing.

GRAPHICAL ABSTRACT



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ABSTRACT

Thermoelectric materials convert waste heat energy efficiently to electricity in an eco-friendly manner. Bi_2Te_3 is a known thermoelectric material, which can convert waste heat and solar energy into electricity in the 200–400 K temperature range. Bi_2Te_3 nanocrystals are prepared in powder form by solvent-free mechanical alloying of elemental Bi and Te powder mixtures under an inert Ar atmosphere. The crystallite size and composition of the Bi_2Te_3 nanocrystals are analyzed using X-ray diffraction, field-emission scanning electron microscope and energy-dispersive X-ray spectroscopy. Thermal and electrical behaviours and the effect of thermal annealing are studied on the 10 h ball-milled sample in a physical properties measurement system in the 30–375 K temperature range. It is observed that the high-temperature thermal annealing induces significant grain growth, reduces lattice strain, along with a reduction of bandgap energy of the mechanically alloyed Bi_2Te_3 nanostructures. Thermoelectric properties and the figure of merit of the nanostructures have improved significantly upon thermal annealing. Enhanced thermoelectric performance of the annealed nanostructures has been explained considering the change in their thermal conductivity, electrical resistivity, and crystallite size induced by thermal treatment.

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