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PAPER

Thermoelectric properties of Sn_2SSe via band engineering with Ge alloying

Baljinder Kaur[1], **Shakeel Ahmad Khandy**[2], **Shobhna Dhiman**[1], **Munirah D Albaqami**[3] and **Kulwinder Kaur**[4]

[1] Department of Physics, Punjab Engineering College (Deemed to be University), Sector 12, 160012, Chandigarh, India
[2] Frontier Research Institute for Interdisciplinary Sciences Islamic University of Science and Technology Awantipora-192122 J&K- India[†]
[3] Department of Chemistry, College of Science, King Saud University, Riyadh, Saudi Arabia
[4] Department of Physics, Mehr Chand Mahajan DAV College for Women, Sector 36, Chandigarh-160036, India
[†] Publisher's note. Whilst IOP Publishing adheres to and respects UN resolutions regarding the designations of territories (available at http://www.un.org/press/en), the policy of IOP Publishing is to use the affiliations provided by its authors on its published articles.'

E-mail: kulwinderphysics@gmail.com and shakeelkhandy11@gmail.com

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Abstract

The thermoelectric properties of Sn_2SSe are investigated via band engineering using Ge alloying. In this work, the electronic and thermoelectric properties of Sn_2SSe doped with Ge at different concentrations (x=0, 0.25, 0.5, 0.75, and 1) are investigated using density functional theory and Boltzmann transport theory. At 300K, the Seebeck coefficient and electrical conductivity are enhanced with Ge alloying from -960μV/K to -1535 μV/K and from 3.4×10^5 S/cm to 4.1×10^5 S/cm respectively. However, the lowest value of lattice thermal conductivity is observed at 700 K which is 2.7W/mK. At x = 1, A remarkably high ZT value 1.7 is achieved at 700 K for $Sn_{2(1-x)}Ge_{2(x)}SSe$. The high ZT value is 1.8 times greater than pure compound.

1. Introduction

Massive amount of waste heat is released into the environment by numerous human activities. The manufacturing process and use of coal, gas, and oil are releasing greater amounts of carbon dioxide. Greenhouse gases are added to the atmosphere due to the burning of fossil fuels and deforestation. Due to the global energy and environmental crisis, energy resources are required that are more efficient, clean, and capable of converting waste heat into usable energy. Thermoelectric (TE) materials have garnered a lot of attention, especially in the past few decades due to their potential to transform waste heat into electricity [1, 2]. The efficient performance of thermoelectric devices is heavily reliant on the power factor and thermal conductivity. The efficiency of any thermoelectric material is characterized by a figure of merit which is given by [3, 4]

$$ZT = \frac{S^2\sigma T}{(\kappa_l + \kappa_e)}, \tag{1}$$

where S is the Seebeck coefficient, σ is electrical conductivity, T is absolute temperature, κ_e is electronic thermal conductivity and κ_l is lattice thermal conductivity. The selection of an ideal thermoelectric material relies not only on its high figure of merit (ZT) but also on factors such as eco-friendliness and cost-effectiveness.

The search for efficient thermoelectric materials is a vibrant area of research driven by the growing demand for sustainable energy technologies and waste heat recovery systems. Continuously exploring new materials and strategies to enhance the thermoelectric performance of existing materials is crucial [5–9]. Chalcogenides encompass a broad class of compounds that contain chalcogen elements (sulfur, selenium, or tellurium) bonded to other elements. Among these compounds, binary chalcogenides [10], ternary chalcogenides [11] and quaternary chalcogenides [12, 13], and other chalcogenides based compounds[12, 14] are particularly noteworthy due to their diverse properties and potential applications. Over the past few years, layered structure compounds have been known for various applications in electronic components, energy storage, piezoelectric

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