Materials Science in Semiconductor Processing 171 (2024) 107995

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp

First principle examination of two dimensional rare-earth metal germanide halides Y_2GeX_2 (X = Cl, Br, I) for thermoelectric applications

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ARTICLE INFO

Keywords:
Thermoelectricity
Rare earth elements
Two dimensional layered materials
Lattice thermal conductivity
Figure of merit

ABSTRACT

In the present work electronic, structural and thermoelectric properties of newly designed layered rare-earth metal germanide halides such as Y_2GeX_2 (X = Cl, Br, I) are investigated. These materials are indirect band gap semiconductors with narrow band gap 0.30 eV for Y_2GeCl_2,0.36 eV for Y_2 $GeBr_2$, and 0.41 eV for Y_2GeI_2 respectively. First principles method along with Boltzmann transport equations (BTE) is utilized together to analyse the thermoelectric properties. These materials are dynamically and mechanically stable. Thermoelectric coefficients such as electrical conductivity, seebeck coefficient and thermal conductivity are computed and put together to ultimately get the Figure of merit (ZT). Y_2GeI_2 has highest figure of merit (ZT) of 0.42 with Seebeck coefficient 532.12 VK^{-1}, electrical conductivity 8.6 $\times 10^5$ Sm^{-1} and has lowest lattice thermal conductivity value of 5.55 Wm^{-1} K^{-1} among three materials, which is necessary to achieve high figure of merit. The computed value of Figure of merit 0.07, 0.22 and 0.42 for Y_2GeCl_2, Y_2GeBr_2 and Y_2GeI_2 accordingly, shows that these materials can be considered as good candidates for energy harvesting in thermoelectric applications.

1. Introduction

Thermoelectrics contributes to revive the waste heat energy from various resources. This scalable technology generate power via direct conversion of heat into electricity through Seebeck effect or provide active cooling under current flow through Peltier effect [1,2]. The Conversion process involves heat and Charge transport, with electrons and phonons mainly being the carriers, thus unraveling the thermal and electronic transport properties of a thermoelectric materials. The efficiency of conversion is characterized by dimensionless quantity Figure of merit (ZT) as per the given relation-

$$ZT = \frac{S^2 \sigma T}{\kappa} \quad (1)$$

where S, σ, T, and κ ($\kappa = \kappa_e + \kappa_l$) refers to seebeck coefficient, electrical conductivity, temperature, and thermal conductivity (κ_e = electronic thermal conductivity, κ_l = lattice thermal conductivity), respectively. The complicated relationships between these variables make it challenging to determine an effective ZT value. Yet, researchers from all over the world use multitude of approaches to enhance the value of ZT [3]. These techniques include band engineering, nanostructuring, dimensionality reduction and various other methods. Although, the main contributors to thermoelectric applications [4–6] have been three-dimensional (3D) materials, however graphene has opened the door for researchers to investigate low-dimensional materials [7]. In contrast to its 2D counterparts, where a new parameter, the length scale, has been introduced, the thermoelectric properties of bulk materials exhibit complex interdependence on one another [8]. Due to large surface area of 2-dimensional (2D) materials relative to 3-dimensional (3D) bulk materials, these materials have distinctive physical and chemical properties [9]. Two-dimensional material with one of the most attractive band structures and extraordinarily high carrier mobilities is graphene. A layer of graphene was created on a piece of scotch tape by Andre Geim and Konstantin Novoselov as they studied the characteristics of graphite [7–10]. A layer of carbon atoms makes up the

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https://doi.org/10.1016/j.mssp.2023.107995
Received 17 August 2023; Received in revised form 15 November 2023; Accepted 16 November 2023
Available online 27 November 2023
1369-8001/