Solid State Communications 363 (2023) 115103

Contents lists available at ScienceDirect

Solid State Communications

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

Properties of the double half-heusler alloy $ScNbNi_2Sn_2$ with respect to structural, electronic, optical, and thermoelectric aspects

H. Mekki [a,b], H. Baaziz [a,b,*], Z. Charifi [a,b], T. Ghellab [a,b], A.E. Genç [c], Ş. Uğur [c], G. Uğur [c]

[a] Department of Physics, Faculty of Science, University of M'sila, 28000, M'sila, Algeria
[b] Laboratory of Physics and Chemistry of Materials, University of M'sila, Algeria
[c] Department of Physics, Faculty of Science, Gazi University, 06500, Ankara, Turkey

ARTICLE INFO

Communicated by L. Brey

Keywords:
Double half-heusler
Optoelectronic
Thermoelectric properties

ABSTRACT

In the current work, the structural, electronic, thermoelectrics, and optical characteristics of the double half Heusler (DHH) $ScNbNi_2Sn_2$ compound are reported for the first time using density functional theory (DFT). The computed band structures show typical semiconductor behavior with an indirect bandgap (0.47 eV) using EV-GGA approximation. We also investigated the optical properties such as the dielectric function, optical conductivity, refractive index. Boltzmann's semiclassical theory attempts to explain a simulation concept in the BoltzTrap software, and the findings were presented and analyzed in terms of electrical conductivity, electronic and lattice thermal conductivities, the Seebeck coefficient, and the Figure of merit over a 50 K–1000 K temperature range. At room temperature, with a low magnitude of lattice thermal conductivity (κ_L) (5.30776 W/m.K) and a maximum value of the merit factor (ZT) is 0.64 at 900 K for $ScNbNi_2Sn_2$ compound is observed. These findings suggest that our material may be a viable option for use in high-temperature thermoelectric devices. We calculated (S, (σ/τ), (k_e/τ)) along the x, y, and z axes utilizing the EV-GGA method. We found out that our compound is thermoelectrically anisotropic. We have also studied in EV-GGA the effect of the carrier concentration on the Seebeck coefficnet at T = 600 K. The maximum value of S is 356.9905 μV/K with $n = 3.04 \times 10^{19} Cm^{-3}$ within GGA and EV-GGA respectively.

1. Introduction

In the last decade, studies into the thermoelectric characteristics of half-Heusler compounds have garnered a lot of interest [1–3]. Multiple examples of advanced thermoelectric materials (YFeSb (Y=Nb, Ta) [4,5], and ZrCoBi [6] are *p*-type transport materials, while TiNiSn [7,8] is *n*-type) included in this group of compounds due to the wide chemical space available to tailor their characteristics. The remarkable electrical transport capabilities of half-Heusler compounds are largely responsible for their outstanding performance [9]. Ternary half-Heusler materials, however, have a disadvantage when compared to the top IV-VI compounds based thermoelectric materials [10,11] owing to their inherently high lattice thermal conductivity (k_L). When compared to other high-performance materials with a half-Heusler formula (T = 300 K), ZrCoBi [6] has a k_L of just 10 W/(m.K), where today's leading thermoelectric material PbTe has an intrinsic k_L of just 2 W/(m.K) [12]. Because of this, it is better to devise a method for locating novel semiconductors that exhibit the electronic characteristics of half-Heusler alloys but have substantially lower k_L.

Although k_L is known to be compositionally dependent via phonon scattering [13,14] and Mechanisms for softening the lattice [6,14], it is also known to be dependent on the size of the primitive unit cell [15]. The value of k_L relies mostly on N which represent the total number of atoms in the elementary unit cell, even for solids with comparable bulk characteristics including Debye temperature, average cell mass, particular thermal capacity, and Gruneisen values [15]. Lower k_L in complex materials with higher N is caused by a lesser percentage of high group velocity (v_g) acoustic modes opposed to smaller (v_g) optical modes. The materials $La_2Mo_2O_9$ ($N = 624$, $k_L = 0.7$ W m^{-1} K^{-1} [16] and $Yb_{14}AlSb_{11}$ ($N = 104$, $k_L = 0.6$ W m^{-1} K^{-1}) [15,17] are two illustrious instances of high N compounds with low k_L values. Nonetheless, N = 3 for ternary half-Heuslers, revealing a vast untapped resource for the discovery of materials with low thermal conductivity if the effective N might be consistently increased. The perovskite type is the basis for a famous group of materials with a wide range of cell sizes [18]. Ternary perovskites ABO_3 (eg, $BaTiO_3$) have $N = 5$, whereas quaternary double

* Corresponding author. Department of Physics, Faculty of Science, University of M'sila, 28000, M'sila, Algeria.
E-mail addresses: baaziz_hakim@yahoo.fr, hakim.baaziz@univ-msila.dz (H. Baaziz).

https://doi.org/10.1016/j.ssc.2023.115103
Received 25 December 2022; Received in revised form 12 February 2023; Accepted 13 February 2023
Available online 17 February 2023