Physica Scripta

PAPER

Tailoring the physical characteristics of $ScTaPd_2Sn_2$ and $ScTaPt_2Sn_2$ double half-Heusler compound for thermoelectric applications

H Mekki[1,2], H Baaziz[1,2], Z Charifi[1,2], T Ghellab[1,2] and I Mili[2]

[1] Department of Physics, Faculty of Science, University of M'sila, 28000 M'sila, Algeria
[2] Laboratory of physics and chemistry of materials, University of M'sila, Algeria

E-mail: baaziz_hakim@yahoo.fr

Keywords: DHH, optoelectronic, mechanic behaviour, ZT

RECEIVED
9 April 2024

REVISED
28 May 2024

ACCEPTED FOR PUBLICATION
12 June 2024

PUBLISHED
21 June 2024

Abstract

Due to its potential uses in thermoelectrics, spintronics, and other sectors, double half-Heusler compounds have recently attracted much attention. This study presents the first-ever report on the structural, electronic, optical, elastic, and thermoelectric characteristics of the double half Heusler (DHH) compounds $ScTaPd_2Sn_2$ and $ScTaPt_2Sn_2$, employing density functional theory (DFT). Using the EV-GGA approximation, the estimated band structures exhibit a semiconductor behavior with an indirect bandgap of 0.549 eV and 0.851 eV, respectively. In addition, we examined optical characteristics. Our material structural stability and stiffness were confirmed using elastic characteristics. Boltzmann's semiclassical theory attempts to explain a simulation concept in the BoltzTrap software. According to the thermoelectric investigation, these DHH are a p-type material, a candidate for thermoelectric application, specifically when doped.

1. Introduction

In a recent study, Anand *et al* proposed the notion of double half-Heusler (DHH) compounds characterized by their enhanced structural complexity, which leads to substantially reduced K_L values, this novel group of half Heusler alloys exhibits many chemical formulas, including double quaternary ($X'X''Y_2Z_2$; $X_2Y'Y''Z_2$; $X_2Y_2Z'Z''$), triple ($X_2'X''Y_3Z_3$), and quadruple ($X'_3X''Y_4Z_4$) [1]. In the context of this investigation, a significant focal point pertains to the quaternary double half Heusler compounds, which exhibit analogous characteristics. These characteristics encompass behaviors to semiconductors, an indirect and narrow band gap, a substantial contribution to the density of states from the d-orbital, mechanical stability, and a Debye temperature of approximately 400 K [2–6]. Furthermore, the researchers Anand *et al* conducted an experimental study to showcase the reduced thermal conductivity (K_L) of the compound $Ti_2FeNiSb_2$, which was synthesized by combining the aliovalent compounds TiFeSb and TiNiSb. The K_L value of $Ti_2FeNiSb_2$ was found to be significantly lower (6–7 W mK^{-1}) compared to that of the compound TiCoSb (25 W mK^{-1}). This reduction in K_L can be attributed to the decreased velocity of phonon groups in the high-frequency range. The recent finding [7] simulated thermal conductivity values of Hf_2Ni_2InSb in its cubic phase range from 13.3 to 3.3 (W mK^{-1}), while in its tetragonal phase, the range is from 12.4 to 2.8 (W mK^{-1}). On the other hand, for the ternary compound HfNiSn, the thermal conductivity ranges from 18.9 to 4.7 (W mK^{-1}) within the temperature range of 300–900 K. The thermal conductivity, denoted as K_L, of Zr_2Ni_2InSb exhibits a range of values between 17.8 to 4.3 (W mK^{-1}) in the cubic crystal structure and 12.1 to 2.9 (W mK^{-1}) in the tetragonal crystal structure throughout the temperature range of 300–900 K. In comparison, the thermal conductivity of ZrNiSn within the same temperature range varies between 18.7 to 4.5 (W mK^{-1}). The previously reported thermal conductivity values at ambient temperature for ZrNiSn and HfNiSn are 19.6 and 18.5 (W mK^{-1}), respectively. In contrast, for Zr_2Ni_2InSb and Hf_2Ni_2InSb in the tetragonal phase, the corresponding values at 300 K are 13.5 and 12.5 (W mK^{-1}), respectively at 300 K [1]. Another illustration from the research we've done in previous periods about the DHH $ScNbNi_2Sn_2$ which has a lower K_L 5.3 (W mK^{-1}). At 300 K and 1.3 (W mK^{-1}) at 1000 K [2] however, a parent ScNiSn has 11.7 (W mK^{-1}) at 300 K [8]