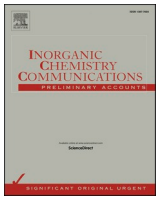
Inorganic Chemistry Communications 170 (2024) 113243

Contents lists available at ScienceDirect

Inorganic Chemistry Communications

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



Short communication

Effect of Pressure on Thermoelectric Performance of Half Heusler Compounds

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ARTICLE INFO

Keywords:
Thermoelectric materials
Density functional theory
half Heusler compounds
Seebeck coefficient
Figure of merit
Pressure

ABSTRACT

In this work, the density functional theory (DFT) combined with Boltzmann transport equations are used to explore the effect of pressure on the structural, mechanical, thermal, and electronic properties of two half Heusler compounds PdXSn (X = Zr,Hf). The electronic band structure is tuned under pressure which enhances the thermoelectric properties of both compounds. The band gap opens with pressure and its value is 0.91 eV (1.26) for PdZrSn and 0.82 eV (1.16 eV) for PdHfSn at 0GPa (30GPa). The indirect nature does not alter at any pressure. The seebeck coefficient enhances from 900 $\mu V/K$ to 1161 $\mu V/K$ for PdZrSn and from 763 $\mu V/K$ to 1012 $\mu V/K$ for PdHfSn at pressure 0GPa to 30GPa. Similar trends observed in case of electrical conductivity and electronic part of thermal conductivity. But the lattice thermal conductivity is reduced from15.16 W/mKto 12.51 W/mK for PdZrSn and from 9.53 W/mK to 8.34 W/mK for PdHfSn at 30GPa respectively. Overall, the figure of merit *ZT* is elevated and attained maximum value of 0.45(0.55) for PdZrSn (PdHfSn) under pressure up to 30GPa.

1. Introduction

Currently, our society is dealing with two major issues: the energy crisis and environmental pollution. Also, fossil fuel depletion has become a more serious issue in daily life. Searching new energy conversion methods that are efficient and environmentally friendly, is especially important. At present, finding clean, renewable energy sources are a major concern for researchers. Thermoelectric conversion technique enables the conversion of heat energy into energy and vice versa,has drawn a lot of attention as an example of clean energy resources. For the past 20 years, scientists have been studying thermoelectricity and looking for new groups of thermoelectric materials. However, the value of thermoelectric efficiency[1–8] ($ZT = \frac{S^2\sigma T}{k}$) for promising thermoelectric materials is still not high Nonetheless, which makes the efficiency of TE devices less competitive than that of existing energy conversion devices.

Due to their unique properties, the Heusler compound families have recently attracted a lot of attention in experimental and theoretical research field. Based on the stoichiometry, Heusler alloys are divided into three groups: (i) half-Heusler[9–15] (XYZ) (ii) full-Heusler [9,16–19] (X_2YZ) and (iii) quaternary Heusler[20–22] (XX_0YZ), in which X, X_0, Y are transition-metal elements and Z is group p elements [19]. Out of these, half Heusler compounds are highly adaptable material due to their simple crystal structures. There are many different forms of Heusler compounds, such as topological insulators, thermoelectric materials, semi-metals, etc. Gautier and his colleagues have discovered their thermodynamic parameters of potential half Heusler materials [23]. Cubic half-Heusler alloys with 18 valence electron and narrow bandgap have high Seebeck coefficients, which makes them suitable materials for thermoelectric (TE) applications. Due to band gap tuneability these materials have aptitude uses in electronics field.

Recent researched have focused on enhancing the *ZT* value through a variety of factors, including electron-hole doping, strain and pressure application, and formation of a layered structure. These techniques have

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https://doi.org/10.1016/j.inoche.2024.113243
Received 31 May 2024; Received in revised form 9 September 2024; Accepted 25 September 2024
Available online 26 September 2024