molecules

MDPI

Article

Electronic Structure-, Phonon Spectrum-, and Effective Mass-Related Thermoelectric Properties of PdXSn (X = Zr, Hf) Half Heuslers

Bindu Rani [1], Aadil Fayaz Wani [1], Utkir Bahodirovich Sharopov [2], Lokanath Patra [3], Jaspal Singh [4], Atif Mossad Ali [5,6], A. F. Abd El-Rehim [5,7], Shakeel Ahmad Khandy [8,*], Shobhna Dhiman [1] and Kulwinder Kaur [9,*]

[1] Department of Applied Sciences (Physics), Punjab Engineering College (Deemed to be University), Chandigarh 160012, India
[2] Solar Thermal and Power Plants Laboratory, Physical-Technical Institute, Uzbekistan Academy of Sciences, Chingiz Aitmatov St., 2, Tashkent 100084, Uzbekistan
[3] Department of Mechanical Engineering, University of California, Santa Barbara, CA 93106, USA
[4] Department of Physics, Mata Sundri University Girls College, Mansa 151505, India
[5] Physics Department, Faculty of Science, King Khalid University, P.O. Box 9004, Abha 61413, Saudi Arabia
[6] Physics Department, Faculty of Science, Assiut University, Assiut 71516, Egypt
[7] Physics Department, Faculty of Education, Ain Shams University, Cairo 11771, Egypt
[8] ZJU-Hangzhou Global Scientific and Technological Innovation Center, School of Micro-Nano Electronics, Zhejiang University, Hangzhou 311200, China
[9] Department of Physics, Mehr Chand Mahajan DAV College for Women, Chandigarh 160036, India
* Correspondence: shakeelkhandy11@gmail.com (S.A.K.); kulwinderphysics@gmail.com (K.K.)

check for updates

Citation: Rani, B.; Wani, A.F.; Sharopov, U.B.; Patra, L.; Singh, J.; Ali, A.M.; Abd El-Rehim, A.F.; Khandy, S.A.; Dhiman, S.; Kaur, K. Electronic Structure-, Phonon Spectrum-, and Effective Mass-Related Thermoelectric Properties of PdXSn (X = Zr, Hf) Half Heuslers. *Molecules* **2022**, *27*, 6567. https://doi.org/10.3390/molecules27196567

Academic Editor: Kun Zheng

Received: 2 September 2022
Accepted: 26 September 2022
Published: 4 October 2022

Abstract: We hereby discuss the thermoelectric properties of PdXSn(X = Zr, Hf) half Heuslers in relation to lattice thermal conductivity probed under effective mass (hole/electrons) calculations and deformation potential theory. In addition, we report the structural, electronic, mechanical, and lattice dynamics of these materials as well. Both alloys are indirect band gap semiconductors with a gap of 0.91 eV and 0.82 eV for PdZrSn and PdHfSn, respectively. Both half Heusler materials are mechanically and dynamically stable. The effective mass of electrons/holes is (0.13/1.23) for Zr-type and (0.12/1.12) for Hf-kind alloys, which is inversely proportional to the relaxation time and directly decides the electrical/thermal conductivity of these materials. At 300K, the magnitude of lattice thermal conductivity observed for PdZrSn is 15.16 W/mK and 9.53 W/mK for PdHfSn. The highest observed ZT value for PdZrSn and PdHfSn is 0.32 and 0.4, respectively.

Keywords: electronic structure; thermoelectric properties; phonon band structure; lattice thermal conductivity

1. Introduction

The ability of thermoelectric (**TE**) materials to convert heat to electrical energy has attracted a great deal of interest and can play a significant part in developing futuristic energy effective materials and devices [1]. Thermoelectric materials are eco-friendly, with no adverse effects on the environment, and are very important in daily life to achieve energy harvesting. The efficiency of **TE** material can be expressed by its figure of merit (**ZT**), which is defined as [2]

$$ZT = \frac{S^2 \sigma T}{k} \tag{1}$$

where S is Seebeck coefficient, σ is electrical conductivity, T is absolute temperature, and k is total thermal conductivity. The total thermal conductivity (k) of crystal is sum of lattice thermal conductivity (k_L) and electronic thermal conductivity (k_{el}). All these parameters are related to each other, so it is difficult to alter the thermoelectric properties independently.

Several techniques, such as electron-hole doping [3,4], strain engineering, forming a layered structures, effect of resonant levels [5], etc., have been used to enhance the