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Effect of strain on the stability, electronic structure and thermoelectric characteristics of (PdXSn, X = Zr, Hf) half-Heusler compounds: a first-principles study

Bindu Rani[1] · Kulwinder Kaur[2] · Shobhna Dhiman[1] · Marutheeswaran Srinivasan[3] · Shakeel Ahmad Khandy[4]

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Abstract
Effect of volume change (i.e. tensile and compressive strain) on the electronic and transport coefficient of PdXSn (X = Zr, Hf) half-Heusler compounds has been discussed in this report. The dynamic and mechanical stability of these compounds and tunability can be achieved via multiple ways (viz, strain engineering, heterostructuring, alloying, chemical doping, intercalation, as well as an external electric field application, etc.). Here, we make use of strain, where stability and band-gap decrease against tensile strain and reverses against compressive strain. Later, the transport parameters (Seebeck coefficient, electrical conductivity, thermal conductivity) variations and figure of merit (ZT) are computed with respect to chemical potential under different strain conditions. At room temperature, tensile strain makes the lattice thermal conductivity preeminent from 15.16 (9.53) W/mK to 19.66 (15.80) W/mK at 12% and -22% strain, which is also confirmed by the phonon dispersions and elastic constant criteria as well. Semiconducting gap of 2.79 (2.36) eV in case of PdZrSn (PdHfSn) compounds is seen and similar enhancement is observed in the case of figure of merit (ZT) from 0.32 to 0.67 for PdZrSn and from 0.4 to 0.75 for PdHfSn under strain. The estimated volume changes reveal that the detailed theoretical investigations of PdXSn with and without strain provide a theoretical platform for experiments and its possible applications in electronic devices and thermoelectricity.

Keywords Electronic structure · Volume expansion · Thermoelectrics · Heusler alloys · Thermal conductivity · Strain engineering

1 Introduction

Thermoelectricity being discovered nearly two centuries ago, has sustained a steady and growing interest among scientists, particularly since the 1950s. This interest was rekindled after the development of semiconductor materials, which offered the potential to significantly improve the efficiency of thermoelectric devices. However, the necessity for an alternative supportable energy sources and efficient energy conversion equipment is driving this growing interest, as

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✉ Shakeel Ahmad Khandy, shakeelkhandy11@gmail.com; Kulwinder Kaur, kulwinderphysics@gmail.com | [1]Department of Physics, Punjab Engineering College (Deemed to Be University), Chandigarh, India. [2]Department of Physics, Mehr Chand Mahaan DAV College for Women, Chandigarh, India. [3]School of Physical Sciences, Amrita Vishwa Vidyapeetham, Mysuru, India. [4]Frontier Research Institute for Interdisciplinary Sciences, Islamic University of Science & Technology, Awantipora 192122, India.