molecules

MDPI

Article

Effect of Strain on the Electronic Structure and Phonon Stability of SrBaSn Half Heusler Alloy

Shakeel Ahmad Khandy [1,*], Ishtihadah Islam [2], Kulwinder Kaur [3], Atif Mossad Ali [4,5] and Alaa F. Abd El-Rehim [4,6]

1 ZJU-Hangzhou Global Scientific and Technological Innovation Center, School of Micro-Nano Electronics, Zhejiang University, Hangzhou 311200, China
2 Department of Physics, Jamia Millia Islamia New Delhi, New Delhi 110025, India; ishtihadahislam@jmi.edu.in
3 Department of Applied Sciences (Physics), Punjab Engineering College (Deemed to Be University), Chandigarh 160012, India; kulwinderkaur@pec.edu.in
4 Department of Physics, Faculty of Science, King Khalid University, Abha 61413, Saudi Arabia; atifali@kku.edu.sa (A.M.A.); alaa.abdelrehim@kku.edu.sa (A.F.A.E.-R.)
5 Department of Physics, Faculty of Science, Assiut University, Assiut 71516, Egypt
6 Department of Physics, Faculty of Education, Ain Shams University, Roxy, Cairo 11771, Egypt
* Correspondence: shakeelkhandy11@gmail.com

Abstract: This paper presents the strain effects on the structural, electronic and phonon properties of a newly proposed SrBaSn half Heusler compound. Since it is stable considering chemical thermodynamics, we tested its strength against uniform strain w.r.t phonon spectrum and it produces a direct bandgap of 0.7 eV. The direct bandgap reduces to 0.19 eV at −12% strain beyond which the structure is unstable. However, an indirect gap of 0.63 eV to 0.39 eV is observed in the range of +5% to +8% strain and afterwards the strain application destabilizes the structure. From elastic parameters, the ductile nature of this material is observed.

Keywords: electronic structure; half Heusler alloys; phonon properties; elastic constants

Citation: Khandy, S.A.; Islam, I.; Kaur, K.; Ali, A.M.; Abd El-Rehim, A.F. Effect of Strain on the Electronic Structure and Phonon Stability of SrBaSn Half Heusler Alloy. *Molecules* **2022**, *27*, 3785. https://doi.org/10.3390/molecules27123785

Academic Editor: Yanlu Li

Received: 18 May 2022
Accepted: 10 June 2022
Published: 12 June 2022

1. Introduction

The search for technologically useful functional and physically interesting materials has recently pushed plentiful suggestions of proposed materials with stimulating properties assured by first-principle calculations. In this regard, electronic structure theory has been extended to propose novel compounds in presumed structural configurations, in search of useful functional materials [1–3]. Zhang et al. within this domain reported 235 compounds to be thermodynamically and electronic structures of 18 additional materials were investigated, seeking potential new material functionalities [4]. Half Heusler (HH) compounds, since their discovery, have expanded to a database of several hundred due to their phenomenal applications such as spin polarization [5–7], thermopower [3,8–14], (anti-ferro/ferro/ferri) magnetism [15–17], superconductivity [18,19] and topological effects [2,19–21]. After shape memory and spintronics, half Heusler compounds are mainly investigated or re-discovered for intriguing thermoelectric properties as some of these materials display larger seebeck and electrical conductivity values [22]. A high ZT of 0.7–1.5 in MNiSn (M = Ti, Zr, Hf) has been reported [9]. Sakurada et al. from first-principle calculations predicted a ZT of 2.68 for KBiBa. Similarly, FeNbSb-based materials always present a ZT value greater than unity [12,23]. While investigating XIrSb (X = Ti, Zr, Hf) alloys by density functional theory methods, figure of merit in p-type doping of XCoSb (X = Ti, Zr, Hf) compounds premediated a ZT value of 1.0 at 1097 K [11,24]. TrIrSb is found to display a maximum ZT = 0.95 at 800 K [8]. In our previous studies, we explored the thermoelectric and phonon properties of PdTaX (X = Al, Ga, In) materials from first-principle calculations with smaller thermal conductivity values [25]. Among quaternary Heuslers,