Physica B 677 (2024) 415698

Contents lists available at ScienceDirect

Physica B: Condensed Matter

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

Strain dependent electronic structure, phonon and thermoelectric properties of CuLiX (X=S,Te) half Heusler compounds

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ARTICLE INFO

Keywords:
Electronic structure
Phonons
Seebeck coefficient
Half Heuslers
Strain effects

ABSTRACT

We report the strain dependent electronic, phonon and thermoelectric properties of Li-based Half-Heusler compounds. A direct bandgap of 1.50 eV (for CuLiS) and 1.03 eV (for CuLiTe) is observed from HSE calculations. CuLiX (X = S,Te) in their conventional structure are mechanically and dynamically stable semiconductors. However, the compression beyond −15 % (for CuLiS) and −10 % (for CuLiTe) destabilizes the crystal structure due to the overlapping of atomic charge spheres. At the same time, expansion above 4 % produces instability in both systems. The maximum value of Seebeck coefficient significantly increases from ~1500 μ/VK in both alloys ~2400 μ/VK in CuLiS and ~2000 μ/VK in CuLiTe after the application of 5 % compressive strain at 300 K. These alloys achieve maximized thermoelectric efficiency via strain engineering, and thus require further experimental research.

1. Introduction

Half Heusler compounds, since their discovery are revered among the multifunctional category of materials as they exhibit interesting properties including spin-charge polarization [1–3], maximized power factors [4–11], magnetism (anti-ferro, ferri, ferro-magnetism) [12–14], superconducting and topological effects [15–18]. Such systems have shown large power factors [19], ultralow thermal conductivities [20] and other socio-economic benefits (non-toxic, low cost) useful for thermoelectric devices and applications. In thermoelectrics, a general criteria of high Figure of Merit (ZT) is an indicator of better performance of any material and hence a maximum ZT value is always a prerequisite. The efficiency of heat conversion into electricity or Figure of merit (ZT) of a material is determined as per the given relation ($ZT = S^2\sigma T/\kappa$); where S, σ, T, and κ ($\kappa = \kappa_e + \kappa_l$) refers to Seebeck coefficient, electrical conductivity, temperature, and thermal conductivity (κ_e = electronic thermal conductivity, κ_l = lattice thermal conductivity), respectively. In experiments, MNiSn (M = Ti, Zr, Hf) alloys reported ZT values in the range of 0.7–1.5 [5] and 1.1–1.5 for FeMSb (M = Nb, Ti) systems [21–23]. Recently, KBiBa and KBiSr alloys were predicted to achieve the ZT = 2.68 and 1.56, respectively [24]. For the same parameter, ZrXPb (X = Ni, Pd, and Pt) compounds reach the values of 1.71, 1.26, and 1.75, respectively [25]. At elevated temperatures, ZT value of 1.54 is predicted for p-type RuTaSb half-Heuslers [18]. However, the efficient ZT value is often attributed to critically low thermal conductivity, large Seebeck coefficient due to multiple reasons like band degeneracy [18], light elemental composition, phonon scattering, flat band presence, etc. [26] In view of this, K. Jia et al. predicted a ZT of 2.65/1.7 in CuLiX(X = Se, Te) using first principles calculations [27]. A. Dey and coworkers reported a ZT of 0.7 in Bismuth based compounds at room temperature [28] and G. Ding et al. presented the better performing MYSb (M = Ni, Pd, Pt) alloys to be appropriate thermoelectric materials [29]. In line with the above statements, we considered the density functional theory-based simulations on a new half-Heusler (CuLiS) and its comparison with CuLiTe. In addition, we studied its chemical, phonon, mechanical stability aspects and electronic properties in general to relate the final conclusive remarks on possible thermoelectric applications as well. We also tried to scrutinize the strain effects on the

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https://doi.org/10.1016/j.physb.2024.415698
Received 30 March 2022; Received in revised form 13 August 2023; Accepted 15 January 2024