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Strain engineering of electronic structure, phonon, and thermoelectric properties of p-type half-Heusler semiconductor

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ABSTRACT

We thoroughly inspected the strain induced electronic properties, phonon dynamics and thermoelectric performance of *ZrRhSb* compound via density functional theory calculations. The optimized lattice parameters are in accord with the experimental observations. The equilibrium lattice constant is utilized to predict the p-type semiconducting and indirect energy gap of 1.15 eV between the X and Γ symmetry points. The application of strain widens the band gap up to 1.5 eV at 10% of compressive strain keeping the indirect nature consistent. Phonon studies display positive frequencies up to 5% of expansion and 25% of compression and thus confirm the dynamic stability of ZrRhSb under strain. Machineability and elastic properties, evidenced from elastic constants and Pugh's parameter characterize it as a ductile alloy while maintaining its Debye temperature to 333 K. Herein, using ab initio quantum mechanical calculations and Boltzmann theory, optimization of thermoelectric performances in strained and robust ZrRhSb phase was performed. Starting from 300 K, it displays satisfactory thermoelectric performances, namely figure of merit $ZT_e > 0.65$ and Seebeck coefficient >190 μV/K. Better performances via strain engineering were obtained at room temperature, where ZT_e values reach 0.81 with a minimal fluctuation over broad temperature spectrum. The optimal strain conditions are achieved at 10% compression, where the S = 426 μV/K and figure of merit reaches up to a maximum of 0.91 at 800 K, which signifies the possible exploitation of ZrRhSb for thermoelectric applications.

1. Introduction

Plentiful Heusler alloys [1–3] discovered with more than 1000 members have entertained much more researchers by being an active research area that tallied new tactics and strategies for inquiring their potential applications. The breakthroughs include the exhibition of high Curie temperature [4,5], robust spin polarization [6,7], low temperature values of saturation magnetization [8,9] and giant anomalous Hall effects [10], etc. intensified their insights for new possibilities of intriguing properties. The devices like thermoelectric generators, tunneling magnetoresistance (TMR), spin injectors or magnetic tunnel junctions have gained momentum in the study of efficiency and durability with the advent of Heusler based new materials [11,12]. The potential feature of electronic structure of such compounds ranges from half-metallicity [13] semiconductor or topological behavior [14,15], which can be utilized for thermoelectric power generation. Power factor ($S^2\sigma T$) or figure of merit ($ZT = S^2\sigma T/\kappa$, here the symbols have their usual meanings) has been an indicative parameter to predict the thermoelectric efficiency of any material. Till date lot more new materials are reported to be thermoelectrically resourceful e.g. p-type PbTe−SrTe reaches the maximum of ZT equal to 2.5 [16], Bi_2Te_3 and Sb_2Te_3 bilayers exhibit ZT = 2.4 [17], whereas SnSe makes it up to 2.6 [18], and $Fe_2V_{0.8}W_{0.2}Al$ with most recent uplift in ZT makes it to 5 [19]. Ti/Sn doped NbFeSb [20] and TaFeSb [21] heuslers are experimetally found to achieve ZT equal to 1.1 and 0.5, respectively. TaIrSn [22], p-type TiPdSn [23], n-type XNiSn [24], p-type Fe(V,Nb)Sb [25] and p-typeXCoSb (X = Ti, Zr, Hf) [26] alloys with high ZTs displaying potential high-temperature TE efficiency are among the few to note down here. Owing to the band degeneracy of Nv = 8 and possibility of engineering the bandstructure rationally as well as via phonons, large ZT values up to 1.5 are achievable in few Fe-based HH alloys [27]. However, different methods and alterations are rigorously putforward to design the more efficinet HH materials so as to deliver an increased capability of waste conversion to direct

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