Assessing the thermoelectric properties of PdScBi half-Heusler alloy

Paul O. Adebambo[1], **Funmilayo Ayedun**[2], **Ridwan O. Agbaoye**[3], **and Gboyega A. Adebayo**[1]

[1]Department of Physics, Federal University of Agriculture, PMB 2240 Abeokuta, Nigeria

[2]Department of Physics, National Open University of Nigeria, Abuja, Nigeria

[3]Applied Science Department, Federal College of Dental Technology and Therapy Enugu, Nigeria

adebambopo@funaab.edu.ng — +2348030825044

Abstract

We will be discussing the results of our probe into the thermoelectric properties of PdScBi Half-Heusler alloy. This was achieved by combing the density functional theory with Boltzmann transport properties and the modified Callaway model. The results of this finding revealed that PdScBi alloy is dynamically stable. Besides, it was observed that this alloy could be used in thermoelectricity.

Introduction

Heusler alloys are a class of numerous intermetallic compounds classified into two types with general composition ABC and A_2BC. The density functional theory, Boltzmann's transport theory, finite displacement method, as well as modified Callaway theory, are used to obtain the thermoelectric properties of PdScBi alloy. Our primary objective was to have a material with a narrow energy bandgap and low thermal conductivity. After which, an effort was made to calculate the power factor, Seebeck coefficient, electrical conductivity, and total thermal conductivity.

Motivation

Heusler alloys have become the subject of intensive experimental and theoretical investigations. These alloys are applicable in micro-electro-mechanical systems, optoelectronic, thermoelectric, and magnetic shape memory [1], amongst the numerous applications. The search for new thermoelectric materials has motivated us to study PdScBi Half-Heusler alloy in order to meet the global energy challenge.

Methods of computations and calculations

The lattice thermal conductivity was obtained using [2]

$$K = \frac{C_V^{aco}}{C_V^{aco} + C_V^{opt}} \times \frac{K_{LA} + K_{TA} + K_{TA^1}}{3} + \frac{C_V^{opt}}{C_V^{aco} + C_V^{opt}} \times K_0 \quad (1)$$

While the electrical conductivity and the power factor were calculated using [3]

$$\sigma = ne\mu \quad (2)$$

$$PF = S^2\sigma \quad (3)$$

Crystal structure and Lattice constant

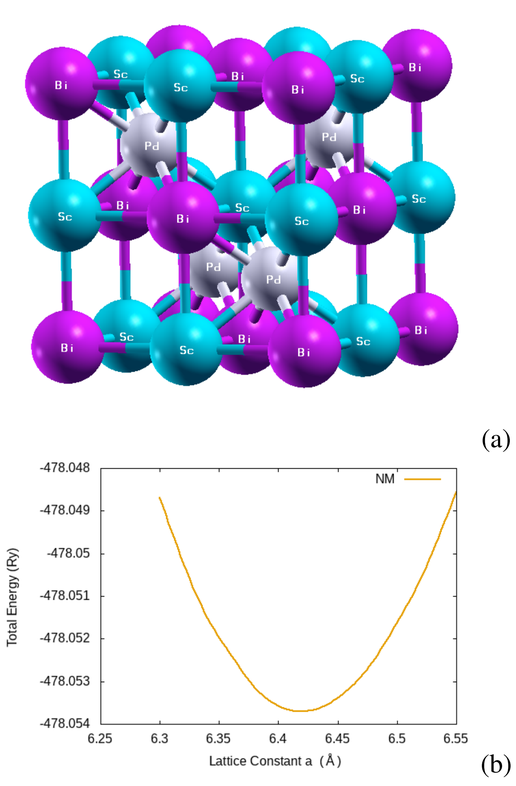

Figure 1: (a)The crystal structure and (b) optimization of the lattice parameters of PdScBi Half-Heusler alloy.

Band Structure and Density of State

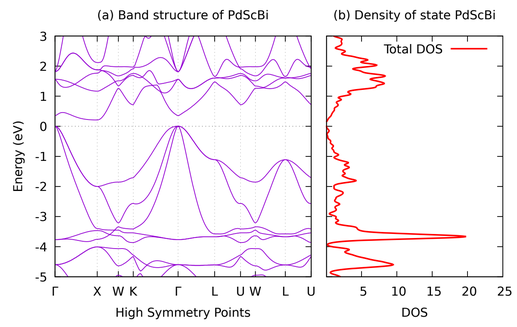

Figure 2: (a) Electronic band structure and (b) Density of state of PdScBi showing an indirect narrow bandgap of 0.31 eV

Phonon dispersion

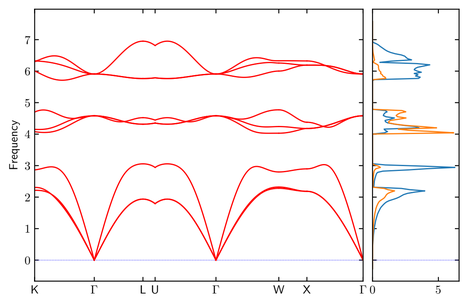

Figure 3: (a)Calculated phonon dispersion curve and (b) VDOS of PdScBi alloy indicating the absence of negative frequency.

Lattice Thermal conductivity

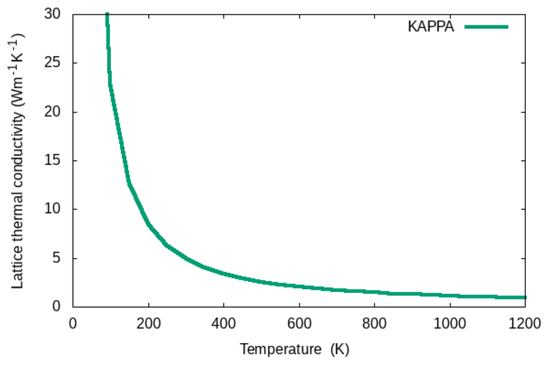

Figure 4: The calcullated lattice Thermal conductivity of PdScBi indicating low conductivity above 200 K.

Thermoelectric properties

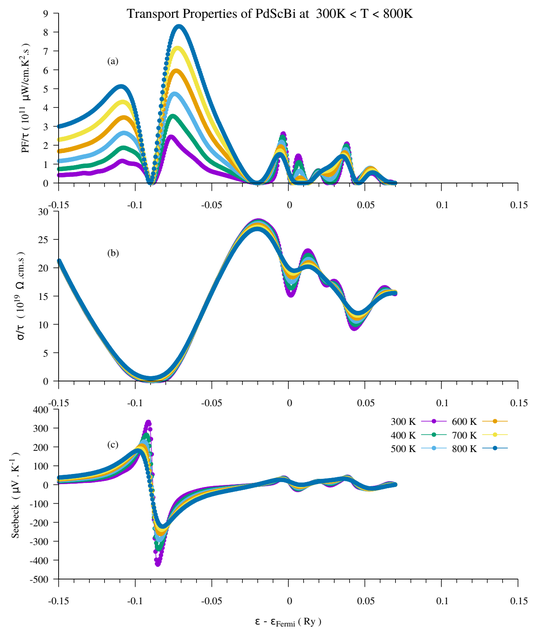

Figure 5: (a) Power factor, (b) Electrical conductivity, and (c) Seebeck Coefficient of PdScBi Half-Heusler alloys where the excellent thermoelectric trait in this material was revealed.

Figure of Merit

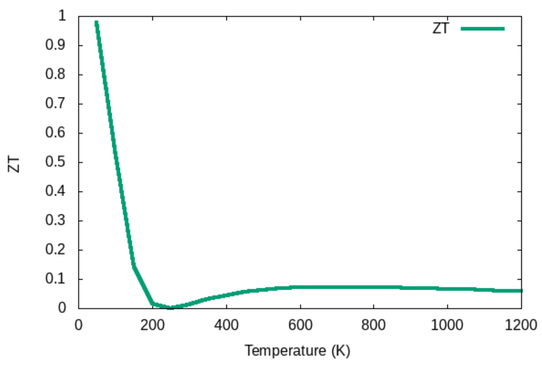

Figure 6: Figure of Merit of PdScBi Half-Heusler alloys.

Conclusions

We have succeeded in using the density functional theory along with other methods as the benchmark to explore the thermoelectric properties of PdScBi alloy. A narrow bandgap of 0.31 eV was obtained. Whereas, at 300 K, the results of the Seebeck in both n and p-type of the material show PdScBi alloy has a promising thermoelectric property. The lattice thermal conductivity of this alloy is low at a temperature above 200 K.

Forthcoming Research

In order to improve/increase the values of the Figure of merit, we will try to dope this alloy with another element.

References

[1] Christian, G. F. B. Siham O. Gerhard H. F. Benjamin B. Xeniya K. Gregory S. Shigenori U. Keisuke K. Claudia F. Sabine W. and Bernd B. *Applied Phys. Letters*, Vol. 98 pp. 252501(2011).

[2] Fan, T., and Oganov, A. R. (2021). AICON2: A program for calculating transport properties quickly and accurately. Computer Physics Communications, 266, 108027.

[3] Adebambo, P. O., Agbaoye, R. O., Bamgbose, M. K., Ayedun, F., Solola, G. T., Adebayo, G. A. (2021). Assessing the structural, electronic, elastic and thermoelectric properties of PtTiSn and PdLaBi transition metal alloys from the first-principles prospective. Materials Science in Semiconductor Processing, 129, 105796.