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High dimensionless figure of merit in full Heusler alloy Ru_2ZrSi: A first principles study

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A R T I C L E I N F O

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A B S T R A C T

We have carried out a theoretical calculation using the full-potential linearized augmented plane-wave method (FP-LAPW), based on density functional theory (DFT) and implemented in the wien2k program to investigate the structural, electronic, elastic and thermoelectric properties of full Heusler alloy Ru_2ZrSi. As the exchange and correlation potential, we used two approximations: the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE) and Tran-Blaha-modified Beck-Johnson approximation (TB-mBJ). The electronic band structures and density of states reveal that Ru_2ZrSi has a semiconductor character with an indirect band gap equals to 0.25 eV and 0.96 eV for GGA-PBE and TB-mBJ approximation respectively. In addition,the mechanical and elastic properties reveal that the Ru_2ZrSi material is mechanically stable, anisotropic and ductile.Moreover, this compound is characterized by high values of the merit factor (ZT) (close to the unity) and Seebeck coefficient (S) which make it promising candidate for thermoelectric applications. It is noteworthy that the present calculationis the first quantitative theoretical prediction of the electronic, elastic and thermoelectric properties for this compound awaiting experimental confirmation.

1. Introduction

Due to the dazzling development of the electronics industry and the quest for increasingly miniaturized electronic components, the international scientific community and industrialists have for several years embarked on the exploration of new concepts, in particular the use of nanomaterial's with proven and predominant quantum effects with excellent ultra-efficient properties and optimal performance, such as perovskites (single and double), full and half Heusler, [1]. The full Heusler with generic formula X_2YZ, where X and Y are transition metals and Z is a group III, IV or V element in the periodic table (Y can also be a rare earth element), are new class of innovative materials dedicated to various technological applications including spintronics and thermoelectric devices [2,3].Recently, large family of materials full Heusler alloys based on ruthenium (Ru) have been investigated experimentally and theoretically due to its interesting properties [4–8]. However, the Ru_2FeGe and Ru_2FeSn alloys exhibit ferromagnetic behavior with an approximate moment as reported by Grover et al. [9]and Patil et al. [10]. The $Ru_2FeSi_{1-x}Ge_x$ alloy series have also been studied experimentally by Deka et al. [11], and they found that these alloys crystallize in the B2 structure while Ru_2FeSi exhibits antiferromagnetic nature, however substitution of Ge at Si sites results in the development of ferromagnetism as x is increased.Subsequently, S. Belhachi [12] studied the structural, electronic and magnetic properties of $Ru_2FeSi_{1-x}Ge_x$ alloys in the generalized gradient approximation (GGA) and it has been shown that $Ru_2FeSi_{1-x}Ge_x$ is stable in a B2 type structure and has a metallic character. Yin and Nash [13]experimentally analysed, using direct reaction and high temperature calorimetry, the Ru_2YZ alloys (Y = Co, Fe, Hf, Mn, Rh, Ti, V, Zr; Z = Al, Ga, In, Si, Ge, Sn) and identified the standard formation enthalpies, lattice parameters and microstructures for these ternary Ru-based Heusler compounds. After that, Yalcin et al. [14] [][][]examined the ground state properties of Ru_2VZ (Z = Si, Ge, Sn) usingthe method of Full-potential linearized augmented plane wave (FP-LAPW) and local orbitals method (FP- LAPW + lo),from this, it was

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