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Determination of mechanical, structural and thermodynamic properties of the half-heusler compound (Zirconium Lead Palladium) in solid state physics

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Half-Heusler compounds are promising semi-conductors which are environmentally friendly and of low-cost thermoelectric materials. They have a high figure of merit. Half-Heusler (HH) alloys are among the most promising novel thermoelectric (TE) materials intended for mid-to-high temperature power generation applications. They are members of the vast family of Heusler alloys with the general composition X_2YZ , consisting of three interpenetrating face-centered cubics (fcc) sub-lattices (Wang et al., 2016). Zirconium Lead Palladium (ZrPdPb) is one of the examples of the Half-Heusler alloy that crystallizes in the face-centered cubic structure with the space group $F4-3m$ (Koller *et al.*, 2009). In this work, the structural, mechanical and thermodynamic properties of ZrPdPb were investigated by the first-principle calculations using Quantum Espresso that implements the Density Functional Theory (DFT). The results indicate that all Half-Heusler compounds are narrow-gap semiconductors. The results of Young's modulus, elastic constants C_{11} , C_{12} and C_{44} , Shear modulus, and Lattice constants, Bulk modulus and pressure derivative which constitute the mechanical and structural properties respectively of ZrPdPb are in good agreement with the results in the literature. The thermodynamic properties of ZrPdPb such as Heat capacity, internal energy, entropy, free energy, Debye temperature etc. were calculated using Quantum Espresso. It is seen that at room temperature i.e. 300K, the internal energy is 23.15kJ/(molk), and the heat capacity is 72.27kJ/(molk). The Debye temperature is found to be 365.3K. From 500K and above, the heat capacity approaches an asymptotic value of 37J/mol/K and obeys Dulong-Petit law which states that at high-temperature Specific heat capacity of a substance remains constant. Also, at sufficiently low temperature, the specific heat capacity is proportional to T^3 . The heat capacity of ZrPdPb shows that the Half-Heusler alloy has little electrical and thermal conductivity as greater heat energy is required to break the intermolecular forces. The mechanical properties ZrPdPb show that the material is not stable under heavy vibration. Suggestions were made to improve the mechanical and thermodynamic properties. Other properties like the magnetic and optical properties of ZrPdPb should be studied. The electrical, mechanical and structural properties of ZrPdPb should be studied by alloying. The electronic, mechanical, structural, magnetic properties of ZrPdPb should also be studied under pressure.

Biography

Ogundola Sunday hails from Irele LGA, Ondo State of Nigeria. He bags BSc Ed in physics from Obafemi Awolowo University, Ile-Ife, Nigeria. He has MSc in Theoretical Physics from University of Benin, Nigeria. He has written some reputed the University-based journals in Nigeria. He is currently a Physics Lecturer at Federal College of Education, Eha-Amufu, Enugu state, Nigeria. He is eagerly opting for his PhD in University of Benin, Nigeria. He is happily married with three children.

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