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THE EFFECTS OF PRESSURE ON THE STRUCTURAL, ELECTRONIC AND MECHANICAL PROPERTIES OF THE HALF HEUSLER COMPOUND NbRuSb

[1]Okunzuwa I.S. and [1]Iyorzor B.E.

[1]Department of Physics University of Benin, Benin City Nigeria

Abstract

The electronic, structural and mechanical properties of Niobium, Ruthenium and Antimony (NbRuSb) has been calculated using density functional theory from first principles calculation (Quantum Espresso). The band structure revealed that Niobium, Ruthenium and Antimony (NbRuSb) is a half heusler and half metal material due to the dual behavior, whereby it acts as a metal as well as a semiconductor. The effects of temperature changes on the Seebeck coefficient, electrical and electronic properties, lattice and thermal conductivity have been calculated. These materials have been identified as good thermoelectric materials with narrow band gaps and flat electronic bands in the valence band. The Seebeck coefficient and electronic thermal conductivity are known to increase with temperature, while the electrical conductivity and lattice thermal conductivity decreased as the temperature increased.

***Keywords*:** Half Heusler, Semiconductor, Electronic Properties, Mechanical properties

1.0 Introduction

Heusler compounds have attracted much interest due to their important application in spintronics, optoelectronics and thermo electrics. Semiconducting half heusler materials are also used in thermoelectric applications, where these materials have a thin electrons in their valence bands and a small band gap. These materials are represented in XYZ form, where X and Y transition metals and the Z element belongs to group III~IV.

These materials are promising materials for use in spintronics and thermoelectric applications because of their narrow band gap at the Fermi level and the voids in these compounds.

In general, Materials are considered based on electronic band structure as Metals, Insulators and Semiconductors, Semimetals, half metals. Materials or substances which allow electricity to flow through them are known as Metals. On application on electric field, They conduct electricity because they allow electrons to flow easily inside them from atom to atom as a result of an overlap between the conduction band and the partially filled valence band. A metal may be a pure chemical element such as gold, or an alloy of variable composition such as stainless steel. In Physics, a metal is generally regarded as any substance capable of conducting electricity at a temperature of absolute zero [1]. In astrophysics, the term 'metal' is cast more widely to refer to all chemical elements in a star that are heavier than the lightest two, hydrogen and helium, and not just traditional metals. Semiconductors are materials which have a conductivity between conductors (generally metals) and nonconductors or insulators (such as most ceramics). Semiconductors can be pure elements, such as silicon or germanium, or compounds such as gallium arsenide or cadmium selenide. In a process called doping, small amounts of impurities are added to pure semiconductors causing large changes in the conductivity of the material. The most commonly used semiconductors are silicon (Si) and Gallium Arsenide (GaAs). A semiconductor material has an electrical conductivity value falling between that of a conductor, like copper, gold, etc. and an insulator, such as glass. Their resistance decreases as their temperature increases, which is behavior opposite to that of a metal. Their conducting properties may be altered in useful ways by the deliberate, controlled introduction of impurities ("doping") into the crystal structure where two differently-doped regions exist in the same crystal, a semiconductor junction is created. A material in which the electron does not flow freely or the atom have tightly bound electrons whose internal electric charges do not flow freely are known as Insulators. Insulators are non-metallic materials which do not permit flow of electrons [2]. Unlike the semiconductor, the band gap for insulators is large so very few electrons can jump the gap. Therefore, current

Corresponding Author**:** Okunzuwa I.S., Email: ikponmwosa.okunzuwa@uniben.edu, Tel: +2348063034388

does not flow easily in insulators. The difference between insulators and semiconductors is the size of the band gap energy. In insulator where forbidden gap is very large and as a result the energy required by the electron to cross over to the conduction band is practically large enough.

1.1 Density Functional Theory (DFT)

Density-functional theory is one of the most popular and successful quantum mechanical approaches to matter. It is nowadays routinely applied for calculating, e.g. the binding energy of molecules in chemistry and the band structure of solids in physics [3]. First applications relevant for fields traditionally considered more distant from quantum mechanics, such as biology and mineralogy are beginning to appear. Superconductivity, atoms in the focus of strong laser pulses, relativistic effects in heavy elements and in atomic nuclei, classical liquids, and magnetic properties of alloys have all been studied with DFT. DFT owes this versatility to the generality of its fundamental concepts and the flexibility one has in implementing them. [4] In spite of this flexibility and generality, DFT is based on quite a rigid conceptual framework.

To get a first idea of what density-functional theory is about, it is useful to take a step back and recall some elementary quantum mechanics. In quantum mechanics we learnt that all information we can possibly have about a given system is contained in the system's wave function ψ. The Schrodinger equation for calculating the ground state energy of a collection of atoms. In the time independent, non-relativistic approach is given as:

$$H\psi(r_1, r_2, \ldots, r_N) = E\psi(r_1, r_2, \ldots, r_N)$$

2.0 Methodology

Calculations have been carried out using the pseudopotential plane wave method within generalized gradient approximation according to the Perdew-Burke-Ernzerhof (GGA-PBE) method.

In this work, we have used QUANTUM ESPRESSO (QE), an open source first principles code, based on density-functional theory, plane waves, and pseudopotentials along with quasi-harmonic approximation (QHA) to calculate the Mechanical and Electronic properties of Niobium, Ruthenium and Antimony (NbRuSb**)** as well as its density of state. We performed the calculations within local density approximation (LDA) and generalized gradient approximation (GGA) with the recently proposed vers ion for solids. We employed a Monkhorst-Pack 11*11*11 k-points mesh in reciprocal space with a plane wave cut-off energy of 55 Ry to obtain the convergence of the structure.

Quantum Espresso is an integrated suite of computer codes for electronic structure calculations and materials modeling, based on density-functional theory, plane waves, and pseudo potentials (norm-conserving, ultrasoft, and projector-augmented wave). QUANTUM ESPRESSO stands for Open Source Package for Research in Electronic Structure, Simulation, and Optimization, it is freely available to researchers around the world under the terms of the GNU General Public License. Innovation and efficiency are still its main focus, with special attention paid to massively-parallel architectures, and a great effort being devoted to user friendliness. QUANTUM ESPRESSO is evolving towards a distribution of independent and inter-operable codes in the Spirit of an open source project, where researchers active in the field of electronic structure calculations are encouraged to participate in the project by contributing their own codes or by implementing their own ideas into existing codes. Plane Waves Basis Sets For periodic systems, the potential has the property: $V(r+na)=V(r)$ where a is the lattice vector and n is an integer. Using Bloch's theorem [5] the wave function can be written as a product of a cell periodic part and a wave like part $\psi_k(r)=\exp(ik.r)f(r)$ Due to its periodicity *f(r) can* be expanded as a set of plane waves $f(r)=\sum_G u_F \exp(iG.r)$ where (G)are reciprocal vectors. Thus the electronic wave **vector** can be written as $\psi_k(r)=\sum_G u_{(k+G)}\exp(i(k+G).r)$. As in the localized case an infinite number of basis functions would be needed to exactly recreate the real *wave function*. The number of wave functions needed is controlled by the largest wave vector in the expansion. This is equivalent to imposing a cut-off on the kinetic energy as the kinetic energy of an electron with wave vector K is given as

$$E_k = \frac{h^2|k|^2}{2m}$$

In Quantum Espresso, plane waves are employed to carry-out the expansion of each single- electron wave function *1/3k* (r); the number of plane waves included in the expansion is limited by the kinetic cut-off energy (ecutwfc) [6]

Where ***H*** is Hamiltonian operator, ***ψ*** is the wave function of the system, ***E*** is the total energy of the system.

3.0 Results

The result obtained from the application of pressure on the NbRuSb crystal structure is represented in the figure below:

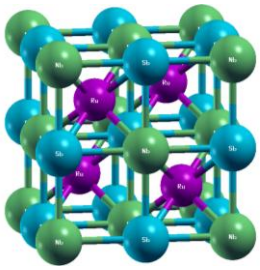

Figure 1: Crystal structure for NbRuSb

The result shows that as pressure increases from 0Gpa to 40Gpa:
1. The crystal structure of the compound remains the same due to hydrostatic pressure applied.
2. The crystal structure is a Faced Centered Cubic structures.
3. The crystal structure is three dimensional

3.1 Electronic Properties

The results obtained from the application of pressure on NbRuSb are presented in the table below.

Table 1: Lattice parameters, Fermi Energy, Band Gap at pressures from 0GPa to 40GPa

PRESSURE (GPa)	LATTICE PARAMETER (a.u.)	FERMI ENERGY (eV)	BAND GAP (eV)
0	11.5194	16.8175	0.4832
10	11.4895	16.9747	0.3294
20	11.3279	17.9111	0.2481
30	11.1927	18.7350	0.1990
40	11.6822	16.8075	0.1765

3.2 Electronic Band Structure and Density Of State

The figures below show the effect of pressure change of the Electronic band structure and the Density of State from 0GPa to 20GPa.

Properties at 0GPa

i. The material is an indirect semiconductor before exerting pressure with the minimum conduction band and the maximum valence band being represented on different Brillion zones. The minimum conduction band occurs at the W zone and the maximum valence band occurs at the L zone.
ii. A band gap of 0.4832eV was achieved.
iii. The 3d- orbital of Niobium makes the most contribution around the conduction band region and the 3d- orbital of Ruthenium makes the most contribution around the valence band region.

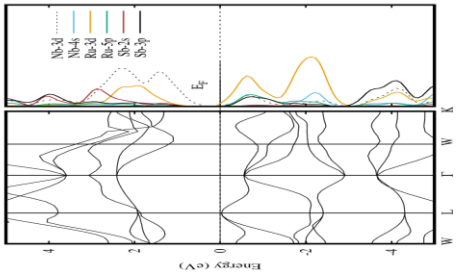

FIGURE 2: Band structure and Density of state of NbRuSb at 0GPa

Properties at 10GPa

i. As the pressure is increased to 10Gpa, the material is an indirect semiconductor with the minimum conduction band at the Γ zone and the maximum valence band at R zone.
ii. A band gap of 0.3294eV was acheived.
iii. The 3d- orbital of Niobium makes the most contribution around the conduction band region and the 3d- orbital of Ruthenium makes the most contribution around the valence band region.

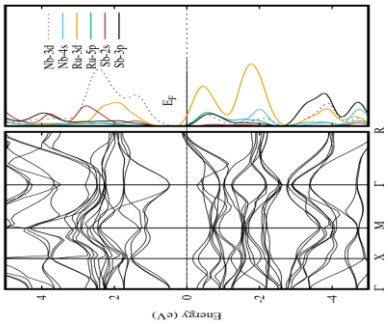

FIGURE 3: Band structure and Density of state of NbRuSb at 10GPa

Properties at 20GPa

i. As pressure is further increased, transition took place which result to a conductor with the minimum valence band at the Γ zone and the maximum valence band at the M zone.

ii. A band gap of 0.2481eV was achieved.

iii. The 3d- orbital of Niobium makes the most contribution around the conduction band region and the 3d- orbital of Ruthenium makes the most contribution around the valence band region.

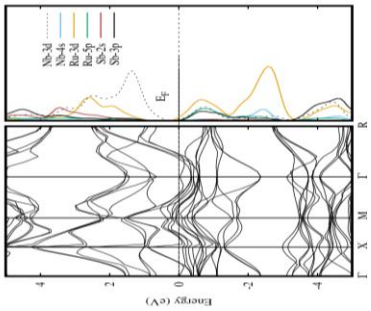

FIGURE 4: Band structure and Density of state of NbRuSb at 20GPa

3.2 Mechanical Properties

The result obtained for the mechanical properties (Bulk Modulus, Young Modulus and Elastic Constant) at each pressure interval (0Gpa to 40Gpa) are represented in the figures below:

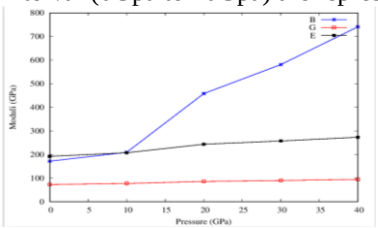

FIGURE 5: A plot of Bulk Modulus (B), Shear Modulus (G) and Young's Modulus (E) against Pressure

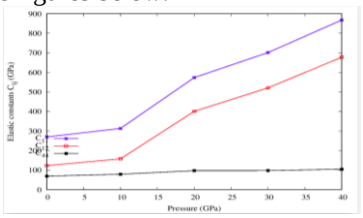

FIGURE 6: A plot of Elastic constants C_{11}, C_{12} and C_{44} against Pressure

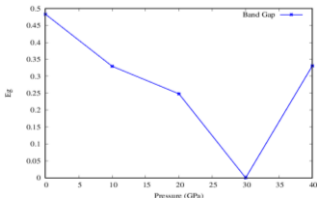

FIGURE 7: Graphical representation of Band Gap (Eg) against pressure

4.0 Conclusion

Calculations of the mechanical and electronic properties of Niobium, Ruthenium and Antimony NbRuSb was carried out using QUANTUM ESPRESSO (QE).

The half heusler compound NbRuSb is a semiconductor, but as pressure increases to 20Gpa, transition took place which result to a conductor.

The results can be applied in the electronic, optoelectronic and spintronic industries which are employed in manufacturing various kinds of electronic devices, including diodes, transistors and integrated circuits. The application of pressure from the results obtained shows that pressure enhances the properties and efficiency of the material for better potential use in applications such as waste heat recovery, radio-isotope thermoelectric generators.

5.0 References

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