

AB INITIO SIMULATION OF THE STRUCTURAL, ELECTRONIC, MECHANICAL AND ELASTIC PROPERTIES OF SOME TRANSITION METALS: YTTRIUM (Yt) AND SCANDIUM(Sc).

Omamoke O. E. Enaroseha^{1*}, Godwin K. Agbajor², O. J. Vwavware³, and Akpoyibo Ogheneovo⁴

^{1,2}*Department of Physics, Delta State University, Abraka, Nigeria*

^{3,4}*Department of Physics, Dennis Osadebay Univeristy, Asaba, Delta State, Nigeria*

**Corresponding author: enarosehaomamoke@gmail.com*

ABSTRACT

We analyzed theoretically from first principle the structural, thermodynamic, electrical and mechanical properties of Yttrium and Scandium. We used the Density Functional theory to provide the solution to the Kohn – Sham equation.

The Xcryden software was used to obtain the structures of the elements studied in correlation within the PBE functions and were treated using the PAW pseudo – potentials and GGA to provide solutions between the core ions and valence electrons.

From the ab initio calculations, we observed that $a(A)$, $B(GPa)$, $B'(GPa)$ and $E(eV)$ for both elements studied are engulf in the structural parameters. Calculations for C_{11} , C_{12} and C_{44} to obtain the mechanical properties and G , B/G , E , μ , A and H to obtain results for the elastic properties were also carried out for both metals.

The results obtained for Scandium shows that the values of B , C' , C_{11} , C_{12} and C_{44} are 51.00, 4.00, 67.00, 43.00 and 32 respectively. For Yttrium we obtained 47.00, 4.07, 53.00, 40.20 and 22.00 corresponding to B , C' , C_{11} , C_{12} and C_{44} respectively. The paper also provides results that agreed qualitatively with experimental data and other theoretical techniques discussed in the literature.

KEYWORDS: Scndium, Yttrium, elastic structural, thermodynamic

1.0 INTRODUCTION

Continuous interest in the study of properties of some transition metals is determined by progressive advances in the theoretical applications to elucidate the nature of the materials and,

on the other hand, by discovering their physical effects. These study also illuminate the nature of materials in the planetary interiors and gain a better understanding of processes in matter in the interest of inertial confinement fusion[1,2,3]. The challenges of understanding the properties of Yttrium and scandium are essential in its effective usage in technological advancement and as such many researchers have carried out series of researches in finding their structural, thermodynamic, electronic, optical and mechanical properties to improve our understanding of these elements and their compounds.[4,5,6,7,8]

One of such studies of scandium compounds carried by Pavas et al[8] elucidates the nature of scandium chalcogenides Structural properties, which are used in the marking of sophisticated materials and glasses. Their results are in the good agreement with the available theoretical and experimental data for lattice constant and bulk modulus values for ScTe, ScS, and ScSe.

The calculated elastic constants by Arikian *et al*[9] for C11, C12 and C44 in L12 phase for ScX3 (X = Ir, Pd, Pt and Pd) compounds were carried using the energy-strain method. They established from their results the metallic character exhibited by all four alloys analyzed through the density of states (DOS) and band structure.

Ekuma *et al*[10] applied the Ab initio technique with the BZW-EF method to study some properties of transition metal mono-nitrides: ScN and YN..

The parameterized exchange correlation contribution by Perdew and Wang were adopted in the generalized gradient approximation (GGA) calculations[11] using the Alder DFTand Ceperley Furthermore, Monteseuro *et al*[12] investigated the properties of yttrium gallium garnet, Y₃Ga₅O₁₂ under hydrostatic pressure, and their mechanical stability analyzed up to 90GPa, their results shows the instability of garnet mechanically when the values are above 84GPa .

The above review literatures stems from the background understanding of quantum theory of solids that stems from the many body problems. This is termed the theory of quantum many body systems.

However, in this reviewed related literatures, it was observed that strict studies of lone scandium and Yttrium are rare. Major studies were carried out having scandium and other elements together as compounds. This is also the same case for the element Yttrium whose studies are also scarce as a lone metal. Their compounds are mostly studied by researchers than their lone element when compared to a vast majority. This study seeks to understand the lone properties of these metals.

2.0 COMPUTATIONAL PROCEDURE.

We follow the formalism of Hohenberg–Kohn theorem, for the single – electron wave function, $\Psi_i[n(r)]$.

$$E(\Psi_i[n(r)]) = E_{known}[n(r)] + E_{XC}[n(r)] \quad (1)$$

To simplify our calculations, we split $E_{known}[n(r)]$ into four contributing terms[13]:

$$E_{known}[n(r)] = -\frac{\hbar^2}{m} \sum_i \int \Psi_i \nabla^2 \Psi_i d^3r + \int v(r)n(r)d^3r + \frac{e^2}{2} \iint \frac{n(r)n(r')}{|r-r'|} d^3r d^3r' + E_{ion} \quad (2)$$

The right hand terms in Eq. (2) are detailed in[13].

Since these solutions are deficient on total functional energy while solving the Schrödinger equation for the wave function, we then invoke the Kohn and Sham[14] equations to solve this difficulty:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + v(r) + V_H(r) + V_{XC}(r) \right] \Psi_i(r) = \epsilon_i \Psi_i(r) \quad (3)$$

V , V_H , and V_{XC} are three potentials summed in the Kohn–Sham equations[14]

The Hartree potential is:

$$V_H(r) = e^2 \int \frac{n(r')}{|r-r'|} d^3r' \quad (4)$$

The true form of the exchange-correlation functional guaranteed by the Hohenberg–Kohn theorem, is simply not known[13].

3.0 METHODOLOGY

The solution of eqn (2) [14] within the DFT as implemented in Quantum Espresso Code[15] was used to accomplish first principle calculations. Projected – Augmented Wave (PAW) and pseudopotentials were used to characterize the interaction between core ions and valence electrons. Because of their precision, we used the PAW pseudopotentials and Generalized Gradient Approximation (GGA) to treat the exchange-correlation function within the Perdew-Burke-Ernzerhof (PBE) functional. The pseudo potentials used is **Ge.pbe-kjpaw.UPF**.

The crystal structure of elements considered in this research is simple cubic with a space group F43m at atomic position (0.50 0.50 0.50). The Kohn – Sham single – particle functions were expanded on a basis of plane-wave set with a kinetic energy cut-off of 38.22 Ry for Ge and. This cut-off energy was determined by by running series of consistent calculations for different values of kinetic energy cut-off starting from 50 Ry to 100 Ry at intervals of 5Ry. Irreducible k-points

were equally generated according to the Monkhorst-pack scheme and Brillouin- zone was sampled with 6x6x6, 7x7x7 and 8x8x8 k-point meshes for MnPtSb, MnCoSb and MnNiSb respectively to get the well converged ground state energy. Finally, we tested parameters carefully to ensure that our calculations were accurate. In order to obtain the equilibrium lattice constant, bulk modulus and it's pressure derivative, the E – V results obtained from the calculations were fitted to the second order Birch-Murnaghan equation of state. The validity of the lattice constant, bulk modulus and the calculated band gap were compared with other theoretical results and available experimental data.

Within the validity of Vegard's law, we have for the lattice constant, a, bulk modulus, B and energy gap(E_g) :

$$a(x) = 0.305x + 5.442 \quad (5)$$

$$B(x) = 74.6 - 16x \quad (6)$$

and $E_g(x) = 2.077 - 0.963x \quad (7)$

where x is the alloy composition over range $0 \leq x \leq 1$.

The elastic properties for the cubic solid were computed from the following relations:

$$C_{11} = \frac{3B+4C'}{3} \text{ and } C_{12} = \frac{3B-2C'}{3} \quad (8)$$

$$A = \frac{2C_{44}}{C_{11}-C_{12}} \quad (9)$$

$$G = \frac{G_V+G_R}{2} \quad (10)$$

where

$$G_V = \frac{2C'+3C_{44}}{5} \text{ and } G_R = 15 \left[\frac{6}{C'} + \frac{9}{C_{44}} \right]^{-1} \quad (11)$$

$$E = \frac{9BG}{3B+G} \quad (12)$$

$$\mu = \frac{3B-2G}{6B+2G} = \frac{3B-E}{6B} \quad (13)$$

$$H = \frac{1-2\mu}{6+\mu} \quad (14)$$

Where C' is the shear elastic constant, A is the elastic anisotropic parameter, G is the shear modulus or modulus of rigidity, G_V is the Voigt shear modulus, G_R is the Reuss shear modulus, E is the Young's modulus, μ is Poisson's ratio and H is hardness of the material. C₁₁, C₁₂, and C₄₄ are the three independent elastic constants. Equation (5) through (14) are due to Saini *et al.*[16]

Where C', A, G, G_V, G_R, E, μ and H corresponds to the shear elastic constant, elastic anisotropic parameter, modulus of rigidity or shear modulus, Voigt shear modulus, Reuss shear modulus, Young's modulus, Poisson's ratio and hardness of the material respectively. C₁₁, C₁₂,

and C44 are the three independent elastic constants. Equation (5) through (14) are due to Saini *et al.*[16]

3.0 THEORETICAL ANALYSIS AND PRESENTATION OF RESULTS

The calculated results obtained from the first principle consideration of two transition elements Scandium and Yttrium using DFT within the PBE GGA method as implemented in quantum espresso are presented and discussed in section 4.1 to section 4.4.

4.1. Structural properties

Table 4.1 lattice parameter, bulk modulus and its pressure derivatives

Properties		Scandium	Yttrium
a(A°)	Present work	4.62	4.54
	Experiment and other calculations	4.635	4.558
B(GPa)	Present work	51.00	47.00
	Experiment and other calculations	49.21 [16]	46.9 [16]
B'(GPa)	Present work	270	78
	Experiment and other calculations	281 [13]	79 [13]
E _f (eV)	Present work	520	510
	Experiment and other calculations	531 [13]	511 [13]

Scandium (Sc) and Yttrium (Y) transition elements crystallize in the Fm3m structure with space group F432 and their structures are shown in Fig 4.1 and 4.2 respectively. The input file for each of these elements was uploaded into the Xcryden package to generate the structure of the elements.

Fig 4.1: Structure of Scandium

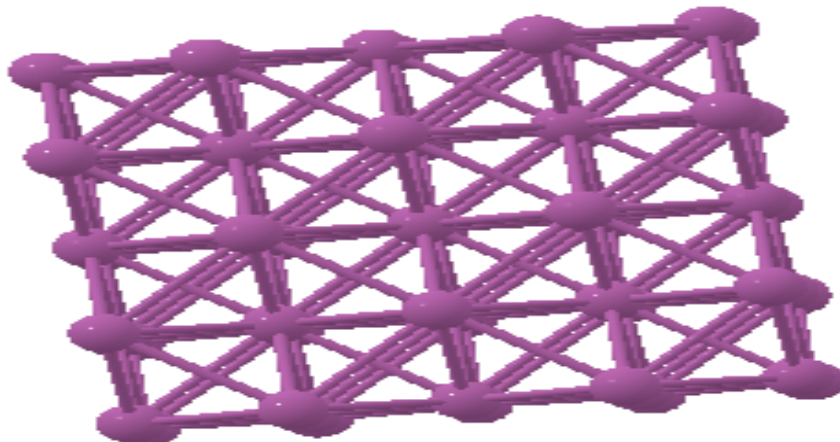


Fig 4.2: Structure of Yttrium

By fitting the computed results for a range of lattice parameters $(-0.3x + 0.3)$ in steps of 0.1 (where x is an experimental lattice parameter value), we were ascertain from Table 4.1 the convergence of the lattice constant to the third order of Birch – Murnaghan equation of as given in the form[17]

$$E_v = E_0 + \frac{9BV_0}{16} \left\{ \left[\left(\frac{v_0}{v} \right)^{\frac{2}{3}} - 1 \right]^3 B' + \left[\left(\frac{v_0}{v} \right)^{\frac{2}{3}} - 1 \right]^2 \times \left[6 - 4 \left(\frac{v_0}{v} \right)^{\frac{2}{3}} \right] \right\} \quad (15)$$

Increase in molar mass of the 4d electron and the lattice constant of the compound was observed in this work as in the trend observed in Srikrishna and Sbradhip[18] but not so for the atomic radii since all 4d electron has the same atomic radii of 135 pm. The result for the lattice parameter which deviates from experimental and theoretical results with approximately 1.5% for Sc and 1.8% for Yt. Both elements can be said consistent with previous reports. The bulk moduli also tally experiments and other reported results.

A sufficient but necessary condition for the ground state thermodynamic stability of half heusler alloys is that the energy of formation is negative i.e at zero temperature, the compound is more stable than its constituent elements. Energy for each alloys can be obtained using the equation below:

$$E_{formation} = E_{Mn} + E_Q + E_{Sb}$$

The negative energy of formation implies that they are both thermally stable and that they can be easily synthesized in the laboratory.

4.2. Electronic properties

Table 4.2

	Scandium	Yttrium
Band Gap	0.0000	0.0000

The band structure and density of states were generated using quantum espresso code and using the cell dimension obtained from the ferromagnetic state of the elements. The zero band gap indicates that these materials are indeed metals with conductivity. Their band structure is as shown in Fig. 4.3 and 4.4 for scandium and Yttrium respectively.

The corresponding density of state shows a peak across the Fermi level indicating an engulfing of the covalent band over the valence band.

Fig 4.3: Band Structure and density of state of Scandium

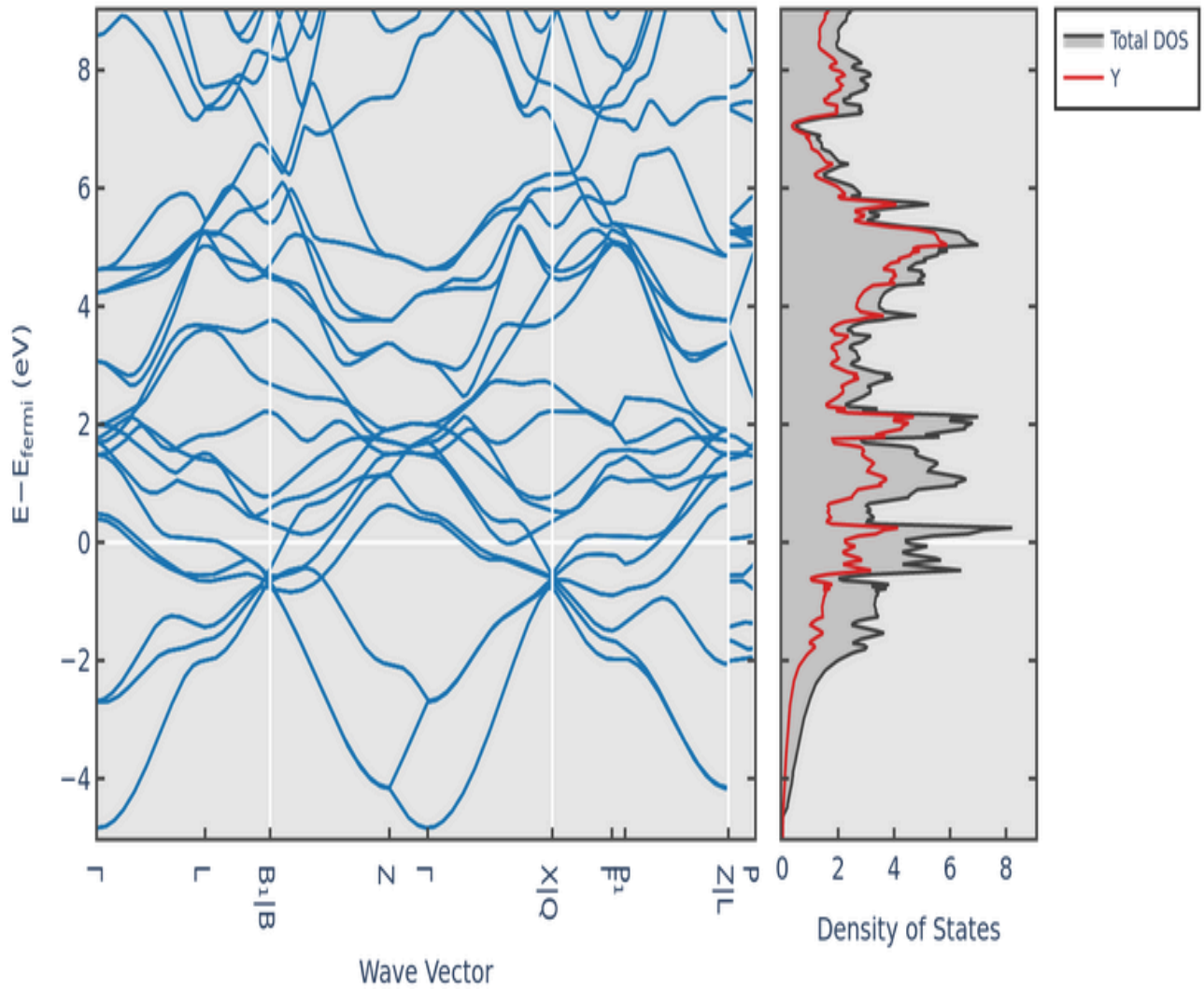


Fig 4.4: Band Structure and Density of state of Yttrium

4.3. Mechanical properties

Table 4.3

Properties		Scandium	Yttrium
C'		4.00	4.07
C ₁₁	Present work	67.00	53.00
	Experiment and other calculations	63.21 [16]	49.30 [16]
C ₁₂	Present work	43.00	40.20
	Experiment and other calculations	42.00 [16]	38.21 [16]
C ₄₄	Present work	32.00	22.00
	Experiment and other calculations	28.21 [16]	21 [16]
C ₁₁ – C ₁₂		24.00	65.80
2C ₁₁ + 2C ₁₂		220	186.40

The link provided by the elastic constant of solids between mechanical and dynamical behaviors of a crystal is quite informative in determining the nature of forces in the solids [16]. The deformation of materials under any small stresses can be characterized by elastic constants and the effects of strain on the electronic properties of the material. The elastic constants of the materials were analyzed, in a bid to establish the mechanical stability of the alloys investigated, and this presented in Table 4.3. These elastic constant offers the criterion for the mechanical stability of the alloy. For an alloy to be mechanically stable, its strain must be positive. This means that the three criteria and conditions [19] must be met. They are $C_{11} - C_{12} > 0$, $C_{44} > 0$ and $C_{11} + 2C_{12} > 0$. Results from this work therefore imply that the elements studied are mechanically stable which is in good agreement with literatures. The parameter C₄₄, C₁₁ – C₁₂ and 2C₁₁+ 2C₁₂ represents the three fold, two-fold degenerate and non-degenerate levels of the bands in the cubic system.

4.4. Elastic properties

Table 4.4

Properties		Scandium	Yttrium
G_v		20.80	14.828
G_R		26.72	7.965
G	Present work	23.76	17.343
	Experiment and other calculations	23.72 [20]	16.120 [20]
B/G	Present work	2.146	2.710
	Experiment and other calculations	2.141 [20]	2.6 [20]
E	Present work	61.70	46.330
	Experiment and Other calculations	60.00 [13]	48.21 [13]
μ	Present work	0.30	0.336
	Experiment and other calculations	0.10 [20]	0.10 [20]
A	Present work	2.67	1.22
	Experiment and other calculations	3.14 [13]	1.88 [13]
H	Present work	0.063	0.052
	Experiment and other calculations	0.055 [13]	0.023 [16]

Elastic parameters

The elastic properties of materials arise from Hooke's law and include the Shear Modulus, Anisotropy, Young's modulus, Poisson's ratio, and Hardness as presented in Table 4.5. The Voigt and Reuss approximation, G_v and G_R of the shear modulus were also presented accordingly. The young's modulus E is the ratio of tensile stress to tensile strain and it measures the stiffness of the material. The values obtained for E in all alloys depicts high level of stiffness and these values are a close proximity to experimental data. Sc is therefore stiffer and also harder than Yt.

Other elastic parameters presented also include; the ratio of the bulk modulus B to shear modulus G ; (B/G). hence the ratio is also called the Pugh's ratio and it determines the ductile/brittle behavior of the material. Ductile/brittle behavior of the materials plays a key role during manufacturing of materials. As we reported recently[21] B/G is critical at 1.75. If $B/G > 1.75$, the material is ductile, otherwise it is brittle. The calculated values of B/G from Table 4.4 implies that Both elements are ductile.

The Poisson's ratio supports ionic bonding for both Sc and Yt since $\mu > 0.26$. The Cauchy pressure defined by $C_{12} - C_{14}$ for Sc suggests a directional covalent bonding since it is negative. An isotropic material has their properties direction – independent, while anisotropic materials are direction dependent[22, 23,24,25,26,27]. In other words, a deviation direction from unity in a material renders it anisotropic. Results shows that Sc is more anisotropic compared to Yt and likely to change its property with the direction of its covalent bonding. Also we can say that it will endure cracking when undergoing experimental growth compared to Yt since its anisotropy extensively deviate from unity than the other. This is of course true as it is also harder and stiffer.

5.0. CONCLUSION

Understanding the properties of Yttrium and scandium are essential in its effective usage in technological advancement and as such many researchers have carried out series of researches in finding their structural, thermodynamic, electronic, optical and mechanical properties to improve our understanding of these elements and their compounds. In this research, we used the first principle calculation to ascertain the properties of these elements in the periodic table and compare the results obtained with already known experimental properties of these element so as to enhance the production, hybridization and doping (on necessary occasions) with other elements in the periodic table.

For the structural properties of these elements, the result for the lattice parameter which deviates from experimental and theoretical results with approximately 1.5% for Sc and 1.8% for Yt. Both

elements can be said consistent with previous reports. The bulk moduli also tally with experiments and other reported results.

Also all results were generated using the quantum espresso code and using the cell dimension obtained from the ferromagnetic state of the elements. The zero band gap indicates that these materials are indeed metals with conductivity. The corresponding density of state shows a peak across the fermi level indicating an engulfing of the covalent band over the valence band.

Furthermore into its mechanical properties, the results from this work therefore imply that the elements studied are mechanically stable which is in good agreement with literatures. The parameter C_{44} , $C_{11} - C_{12}$ and $2C_{11} + 2C_{12}$ represents the three fold, two-fold degenerate and non-degenerate levels of the bands in the cubic system.

And finally for its elastic properties, the results shows that Sc is more anisotropic compared to Yt and likely to change its property with the direction of its covalent bonding. Also we can say that it will endure cracking when undergoing experimental growth compared to Yt since its anisotropy extensively deviate from unity than the other. This is of course true as it is also harder and stiffer.

DEDICATION: Enaroseha dedicate this article in memory of his lovely mother, Mrs. Ichehono Eribo who passed on the 20th of February 2023.

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