

Structural Optimization, Electronic Band Structure, Mechanical and Thermodynamics Properties of Fe₃Al

I. S. Okunzuwa^{1*} and E. Aigbekaen Eddy²

¹*Department of Physics, University of Benin, Benin City, Nigeria.*

²*Department of Physics, College of Natural and Applied Sciences, Igbinedion University Okada, Benin City, Nigeria.*

Authors' contributions

This work was carried out in collaboration between both authors. Author ISO was majorly involved in the write up of the article as well as minor computational input. Author EAE was majorly involved in the computational aspect. Both authors read and approved the final manuscript.

Article Information

DOI: 10.9734/PSIJ/2021/v25i230239

Editor(s):

- (1) Dr. Humaira Yasmin, King Faisal University, Saudi Arabia.
- (2) Dr. Pratima Parashar Pandey, Dr. APJ Abdul Kalam Technical University, India.
- (3) Dr. Lei Zhang, Winston-Salem State University, USA.

Reviewers:

- (1) Sherin Saraireh, Taibah University, Saudi Arabia.
- (2) Pradeep R Varadwaj, The University of Tokyo, Japan.

Complete Peer review History: <http://www.sdiarticle4.com/review-history/67620>

Original Research Article

Received 27 February 2021
Accepted 04 May 2021
Published 12 May 2021

ABSTRACT

We calculated the structural, electronic, mechanical and thermal properties of Fe₃Al semiconducting using Quantum ESPRESSO, an open source first principles code based on density-functional theory, plane waves, and pseudopotentials. Structural parameter results (equilibrium lattice parameters, bulk modulus and its derivative pressure) have been reported. The underestimated band gap is obtained along with higher state density and energy bands around the fermi level. Mechanical properties of the rock-salt structure of Fe₃Al, such as C_{11} , C_{12} , and C_{44} , shear modulus (G), Young's modulus (E), and Poisson's ratio (σ) were investigated. The thermodynamic parameters are also present. The results are in good agreement with the available experimental and other theoretical results.

Keywords: Plane waves; pseudopotential; density functional theory.

*Corresponding author: E-mail: ikponmwosa.okunzuwa@uniben.edu;

1. INTRODUCTION

Metals, any of a class of substances characterized by high electrical and thermal conductivity as well as by malleability, ductility and high reflectivity of light. Approximately three-quarters of all known chemical elements are metals. The most abundant varieties in the earth's crust are aluminium, iron, sodium, potassium, and magnesium. The vast majority of metals are found in ores (mineral bearing substances), but a few such as copper, gold, platinum and silver frequently occur in the free state because they do not readily react with other elements. Metals are usually crystalline solids. In most cases, they have a relatively simple crystal structure distinguished by a close packing of atoms and high degree of symmetry. Typically, the atoms of metals contain less than half the full density of electrons in their outermost shell. Because of these characteristics metals tend not to form compounds with each other.

The high electrical and thermal conductivities of the simple metals (i.e, the non-transition metals of the periodic table) are best explained by reference to the free-electron theory. According to this concept, the individual atoms in such metals have lost their valence electrons to the entire solid, and these free electrons that give rise to conductivity move as a group throughout the solid. In this case, the complex metals (i.e., the transition elements) conductivities are better explained by the band theory which takes into account not only the presence of free electrons but also their interaction with so-called d electrons. The mechanical properties of metals such as hardness, ability to resist repeated stressing (fatigue strength), ductility, and malleability, are often attributed to defects or imperfections in their crystal structure. The absence of a layer of atoms in its densely packed structure, for example, enables a metal to deform plastically, and prevent it from being brittle. [Adam Augustyn, Editors of Encyclopaedia Britannica, 2019].

They can also display desirable magnetic, superconducting and chemical properties, due to their strong internal order and mixed (metallic and covalent / ionic) bonding, respectively. Intermetallic compounds have given rise to various novel material development. High strength-low density, larger electrical resistivity-high melting point etc., are some of the specific properties that enhance the importance of intermetallic compounds. The search for new

materials with improved properties continues, and hence, the study of new materials with improved properties continues, and hence, the study of intermetallic compounds assumes considerable importance. [Schulze, 1967]

2. MATERIALS UNDER STUDY

The comparative study of structural, electronic, thermodynamic and mechanical can be understood to some extent when we take a close look at the individual compound.

2.1 Iron Aluminide (Fe_3Al)

Aluminides of transition metals like nickel, iron, titanium, niobium and cobalt have been widely studied due to their attractive physical and mechanical properties of critical importance in a variety of applications [1]. Among these compounds, iron aluminides are specially interesting due to their low density, low production cost, good mechanical properties and corrosion resistance at high temperatures [2]. Iron aluminides are about 30% lighter than commercial high temperature structural materials like stainless steel and nickel based super alloys [3]. Studies have shown that iron aluminides have good high temperature corrosion resistance in oxidizing and sulfidizing environments [4] found in typical industrial applications like power generation systems. This is attributed to the formation of dense and adherent alumina scales on the surface of the material. Natesan [5] confirmed these observations and concluded that the oxidation rates of iron aluminides in single-oxidant environment (like air or gases with low oxygen potentials) are significantly lower than those for chromia-forming commercial alloys. These properties allow intermetallic compounds in the Fe–Al system to be employed at high temperatures as structural materials, gas filters and heating elements [2]. Two of these compounds, FeAl and Fe_3Al , are considered very attractive due to good strength and corrosion resistance at high temperatures [6].

FeAl, with a B2-ordered cubic CsCl structure, exists over a wide range of aluminum contents (35–50 at. %). The ordered $D0_3$ cubic structure of Fe_3Al is observed around 25 at. % Al and it is stable in the interval 23–36 at. % Al at low temperatures. The region of stability for Fe_3Al $D0_3$ structure tapers off at higher temperatures. Both B2 and $D0_3$ structures are perfectly ordered only when their compositions correspond to the stoichiometric compounds [3]. The high magnetic

permeability shown by Fe_3Al makes it useful as a soft magnetic material.

FeAl has a lower melting point, but a better oxidation resistance. FeAl also has a lower density and higher strength-to-weight ratio compared to steels and super alloys [7]. In addition, it exhibits relatively high electrical resistivity which makes it suitable for use as a heating element [Gedevanishvili, 2002].

Iron aluminides can be produced by powder metallurgical methods involving powder consolidation [8] and sintering, which offer advantages such as net-shape processing and cost-effectiveness. It would be advantageous to start with metal powder mixtures as the consolidation process would be easier and cheaper than using powders of preformed intermetallics. In this context, formation of intermetallics in situ in a heated mixture of metal powders is of considerable interest. Such a process is called Combustion Synthesis, Reactive Synthesis or Self Propagating High Temperature Synthesis (SHS), in which a reaction between the reactant particles is initiated during heating. The reaction is exothermic and the generated heat can be utilized to make the process self-sustaining. Several authors like Munir et al. [9] and Mossino [10] have studied this method which can be used to fabricate near-net shape products. However, porosity levels in SHS products are high and can be minimized by sintering under pressure. Rabin et al. [11] have shown that near full density the grain boundaries.

Gedevanishvili and Deevi [7] conducted dilatometric and DSC experiments up to 1350 °C to study the formation of iron aluminide and the sintering behavior in Fe–40 at.% Al powder mixtures. At a heating rate of 5°C min⁻¹, they observed two exothermic peaks at 560 and 655°C. These peaks were attributed to the formation of Fe_2Al_5 and FeAl respectively. The volume expansion observed in heated discs was linked to the formation of Fe_2Al_5 . The reaction mechanism, expansion rate and product Fe_3Al and FeAl compounds can be obtained during the combustion reaction in a hot press by applying external pressure. Godlewska et al. [12] prepared FeAl (40 at. % Al) intermetallic powders using SHS in a loosely packed mixture of elemental powders. Compacted and sintered powder compacts were densified using hot forming methods. They observed that the strength and ductility of the product at room

temperature were sensitive to grain size and adversely affected by the oxide phase distributed along density were found to be strongly dependent on the heating rate.

Gao et al. [13] also studied the synthesis of FeAl powder mixture. While heating the sample, they observed two successive exotherms in the interval 500–650 °C. These peaks correspond mainly to the formation of Fe_2Al_5 which transforms subsequently to FeAl by reacting with residual iron at higher temperatures. The authors have described the formation of pores during different stages of heating and noted the swelling of the sintered product to be quite significant.

Kang and Hu [14] studied the reactive sintering of Fe–Al compacted discs and found that the large swelling observed is mostly due to the formation of Fe_2Al_5 . They suggested that the large thermal expansion is due to the rapid release of exothermic heat from several reactions occurring simultaneously within the sample, followed by a shrinkage due to heat dissipation. Large differences in the solid solubilities, melting points and diffusion rates [Godlewska, 2003] for the components lead to the development of pores which cause swelling in the sample.

Pochec et al. [15] have suggested a two-step mechanism for the formation of iron aluminides in Fe–50 at. % Al powder mixtures. They report the formation of two aluminum-rich phases FeAl_3 and Fe_2Al_5 due to a slow diffusion process at temperatures below 615 °C. The SHS reaction initiates above this temperature resulting in the formation of ordered FeAl phase together with the fragile FeAl_2 compound. FeAl is obtained as the final product after an additional homogenizing process [16].

In a Fe–Al diffusion couple study, Wang and Wood [17] found that FeAl_3 was dominant on the iron side of the Fe–Al interface at 600°C, highlighting the diffusion of aluminum into iron grains. Intermetallic compound formation was also observed to be significant at the iron grain boundaries, confirming the higher mobility of aluminum atoms along the iron grain boundaries. They also observed the formation of Fe_2Al_5 above the melting point of aluminum through the diffusion of iron into aluminum.

Although, thermodynamic data indicate the formation of FeAl_3 before Fe_2Al_5 , in general, Fe_2Al_5 forms as the major phase at the interface

between aluminum and iron particles due to kinetic factors [18]. It may also be noted that the growth parameter is much larger for Fe_2Al_5 relative to FeAl [Naoi, 2007].

The present study aims to continue the efforts to understand the key aspects of reactive synthesis of iron aluminides from elemental powder mixtures. The effect of processing variables including particle size of reactants and heating rates have also been studied. The synthesized products have been characterized using scanning electron microscopy, energy dispersive spectroscopy and X-ray diffraction methods.

2.2 Preparation

The reaction between Al and Fe to generate iron aluminide is exothermic. Production from direct melting of Al and Fe is economical, but any water in the charge produces issues with the generation of hydrogen which shows solubility in the iron aluminide, leading to gas voids. Blowing with argon or vacuum melting alleviates this. [Sikka and Vinod, 1994]. Coating of iron aluminide can be prepared by chemical vapor deposition onto iron. [John, Sundararaman, 2013].

Potential uses for iron aluminides: electrical heating elements, piping and other work for high temperature process including piping for coal gasification and for super heater and re – heater tubes. [Sikka and Vinod, 1994]. It has also been suggested as structural material for lunar use. [Landis and Geoffrey, 2006]

2.3 Scope and Objectives of the Present Work

In the present work, we have optimized and studied the crystal structure of compound Iron Aluminide along with its band structures. From the calculation of band structure one can have idea of the band gap energy of given metals and semiconductors. The main objectives of the present work are:

- To study the structural, electronic and mechanical properties of Fe_3Al .
- To study the thermo dynamical properties of Fe_3Al

2.4 Method of Approach

By using the density functional theorem, we have studied the structural and electronic properties of

Fe_3Al based on the generalized gradient approximation (GGA). At first we optimized the parameters such as the k-point grid, kinetic energy cutoff. Then we optimized the lattice parameters by minimization of energy. We studied the band structure.

3. METHODOLOGY

3.1 Computational Details

The theoretical calculations of this work are performed using Quantum Espresso (Quantum open-Source Package for Research in Electronic Structure, Simulation and Optimization) package.

3.2 The Quantum Espresso Program

QUANTUM ESPRESSO is an integrated suite of computer codes for electronic structure calculations and materials modeling based on density-functional theory, plane wave basis sets and pseudo potentials to represent electron-ion interactions. QUANTUM ESPRESSO is free, open-source software distributed under the terms of the GNU General Public License (GPL) [<http://www.gnu.org/licences/>].

The two main goals of this project are to foster methodological innovation in the field of electronic-structure simulations and to provide a wide and diverse community of end users with highly efficient, robust, and user-friendly software implementing the most recent innovations in this field. Other open-source projects [Gonze X et al, 2002 and Daniel Crawford et al, 2007.] exist, besides QUANTUM ESPRESSO that address electronic-structure calculations and various materials simulation techniques based on them. Unlike some of these projects, QUANTUM ESPRESSO does not aim at providing a single monolithic code able to perform several different tasks by specifying different input data to the same executable. Our general philosophy is rather that of an open distribution, i.e. an integrated suite of codes designed to be interoperable, much in the spirit of a Linux distribution, and thus built around a number of core components designed and maintained by a small group of core developers, plus a number of auxiliary/complementary codes designed, implemented, and maintained by members of a wider community of users. The distribution can even be redundant, with different applications addressing the same problem in different ways; at the end, the sole requirements that QUANTUM ESPRESSO components must fulfil

are that: (i) they are distributed under the same GPL license agreement [<http://www.gnu.org/licenses/>] as the other Q UANTUM ESPRESSO components; (ii) they are fully interoperable with the other components. Of course, they need to be scientifically sound, verified and validated. External contributors are encouraged to join the Q UANTUM ESPRESSO project, if they wish, while maintaining their own individual distribution and advertisement mode for their software (for instance, by maintaining individual web sites with their own brand names [Mostofi, Yates and Lee, 2008]). To facilitate this, a web service called *qe-forge* [<http://qe-forge.org>], described in the next subsection, has been recently put in place.

Interoperability of different components within Q UANTUM ESPRESSO is granted by the use of common formats for the input, output, and work files. In addition, external contributors are encouraged, but not by any means forced, to use the many numerical and application libraries on which the core components are built. Of course, this general philosophy must be seen more as an objective to which a very complex software project tends, rather than a starting point.

One of the main concerns that motivated the birth of the Q UANTUM ESPRESSO project is high performance, both in serial and in parallel execution. High serial performance across different architectures is achieved by the systematic use of standardized mathematical libraries (BLAS, LAPACK [Anderson et al, 1999], and FFTW [Frigo and Johnsons, 2005]) for which highly optimized implementations exist on many platforms; when proprietary optimizations of these libraries are not available, the user can compile the library sources distributed with Q UANTUM ESPRESSO. Optimal performance in parallel execution is achieved through the design of several parallelization levels, using sophisticated communication algorithms, whose implementation often does not need to concern the developer, being embedded and concealed in appropriate software layers. As a result the performance of the key engines, PWscf and CP, may scale efficiently on massively parallel computers up to thousands of processors.

QE, based on DFT, implements a variety of methods and algorithms for a chemically realistic modeling of materials from the nano-scale upwards. This package uses a plane waves (PWs) basis set for the expansion of electronic wave function, a pseudopotentials (PPs) to

represent electron-ion interactions and DFT for the description of electron-electron interaction [Nielsen and Martin, 1985]. Some basic computations/simulations that can be performed by this package include:

- Calculations of the Kohn-Sham (KS) orbitals and energies for isolated and extended systems, and of their ground state energies.
- Structural modeling (equilibrium structures of molecules, crystals, surfaces).
- Atomic forces and stresses.
- Ground state studies of magnetic or spin-polarized systems.
- Dynamical modeling (first-principles molecular dynamics) either on the electronic ground state (Born-Oppenheimer) or with fictitious electronic kinetic energy (Car-Parrinello).

Density-Functional Perturbation Theory (DFPT) used in the package to calculate the energy derivatives and related quantities. QE package are used as our first – principles code. QE is a full ab-initio package implementing electronic structure and energy calculation, linear response method (to calculate dielectric constants, Born effective charge and phonon dispersion curves) and third order an-harmonic perturbation theory. It also contains two molecular- dynamics codes, CPMD (Car-Parrinello Molecular Dynamics) and FPMD (First-Principles Molecular Dynamics). Among them, to perform the total energy calculations, PWscf code is used, which used both norm-conserving pseudo potential (PP) and Ultra soft Pseudo-potentials (US-PP) within DFT.

In our case, we use Quantum ESPRESSO integrated module of codes, based on DFT by using plane basis set for expansion of wave function and pseudo potential with required content in first-principle method of calculation to calculate total energies and optimized geometries of compound semiconductors AIAs and GAAs. Also by using this package, band structure is calculated and partial density of states (PDOS) is used to find the nature of material.

3.3 Pseudopotentials and Applications

Generally, single particle wave function is taken into account to solve Kohn-Sham equation in solid on plane wave basis. Due to Wiggling nature of core electron, to express them in plane waves, it requires an extremely large number of basis sets. Since core electron are mostly

localized to ion and are less important in determining physical and chemical properties of the material. Because of this, they can be considered as external effective potential for the valence electrons. However, classification of valence and core electrons on certain atoms may be straight forward. Thus the pseudo-potential method equivalently transforms the all electron problem into valence electron problem only. In our study within QE method we make use of pseudo potentials. The pseudo potential method is an attempt to replace the complication effects of the motion of core electrons and nucleus of an atom with an effective potential term.

4. RESULT AND DISCUSSION

4.1 General Considerations

This paper describes the comparative study of intermetallic alloys such as Fe_3Al . One of the main challenges in first principle calculation is the geometric optimization of structures. We have taken out the energy minimization of Fe_3Al , followed by electronic band structure and density of states. The calculations have being carried out using density functional theory [Watson and Weinert, 1998] using generalized gradient approximation. At first in GGA method, energy minimization is done with respect to lattice

parameter then the same lattice parameter corresponding to the minimum energy state are used to carry out further calculations. In band structure calculations, we plotted the graph of energy versus the high symmetry k-point, and then analyzed the properties of the substance on the basis of band lines and band gap. To view the individual contribution of different orbitals electrons, we study the conduction band edge and valence band edge. In all these self-consistent calculations, we have used the convergence criteria as the difference between energy in the order of 10^{-6} Rydberg.

4.2 Structural Properties

In Fig. 1 below shows the crystal structure of Iron Aluminide (Fe_3Al) with iron atoms in purple colour and aluminum atom in red colours.

The total energies as a function of lattice parameter are fitted to Murnagan equation of state. The equilibrium lattice constant (a), bulk modulus (B_0) and pressure derivative for both Fe_3Al were determined. The result obtained in the present work are presented in Table 1. It can be seen that the results are good with agreements with the available experimental and theoretical values showing that the present work is satisfactory and reliable.

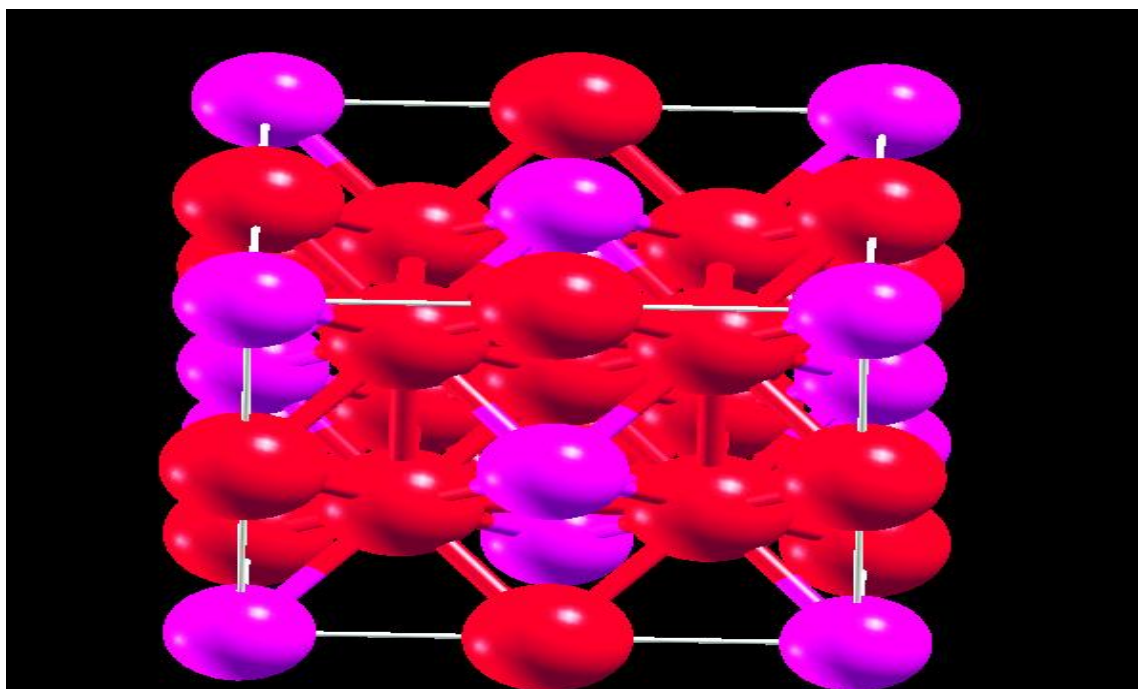


Fig. 1. Conventional cell of the Fe_3Al

Table 1. Structural parameters of Fe₃Al

Material	Lattice Parameter (a) (Å)			Bulk Modulus B ₀ (Gpa)		Pressure Derivative
	Present	Experimental	Others	Present	Other	
Fe ₃ Al	5.31	5.76 (Pearson, 1958)	5.79 (Pearson, 1958)	215.0	159(Pearson, 1958).	4.71

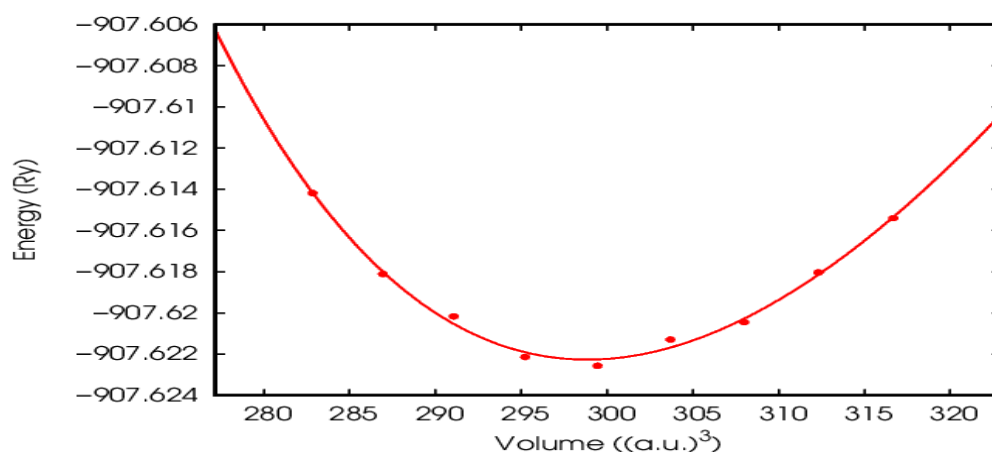


Fig. 2. Graph of volume of Fe₃Al against Energy

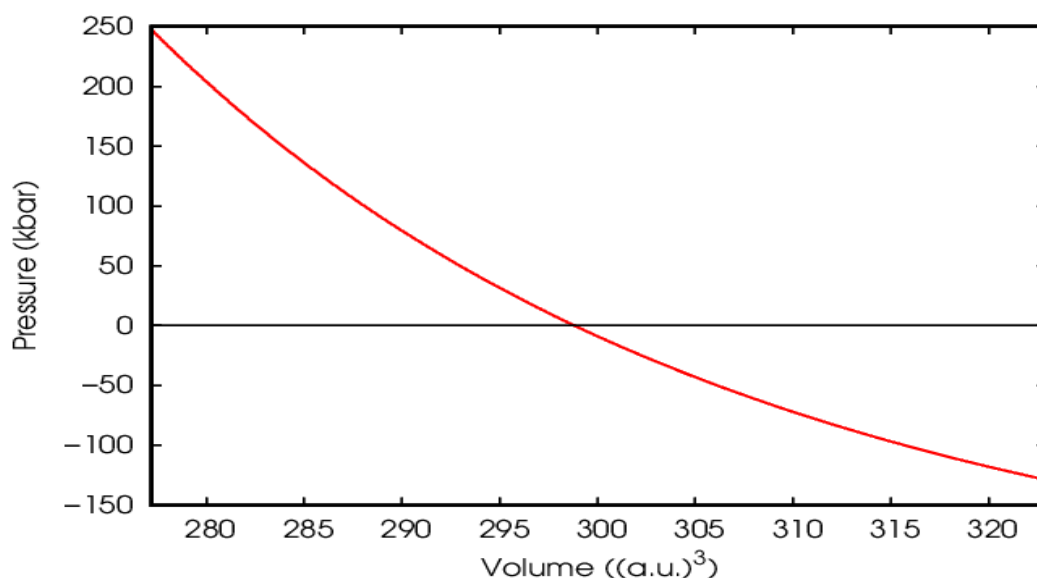


Fig. 3. Graph of volume of Fe₃Al against Pressure

4.3 Mechanical Properties

The mechanical properties of iron aluminide (Fe₃Al) depends on the elastic constants of the compounds which provide an important information concerning the nature of the forces operating in solid materials. The behavior of crystalline materials to an external applied stress

depends on the bulk modulus, shear modulus, Young Modulus, Poisson’s ratio and anisotropy. [Wu et al, 2010]. The values of the elastic constants (C₁₁, C₁₂ and C₄₄), Young’s modulus (E), Poissons ratio (B’) and shear modulus (G) calculated at Voigt approximation, Reuss approximation and the Voigt-Reuss-Hill approximation are presented in the table below;

Table 2. Calculated elastic constant (C_{11} , C_{12} and C_{44}) and Cauchy Pressure ($C_{12} - C_{14}$)

Compound	C_{11} (Gpa)	C_{12} (Gpa)	C_{44} (Gpa)	$C_{12}-C_{44}$ (Gpa)
Fe ₃ Al	278.69530	203.616332	136.851711	141.843639

Table 3. Voigt-Reuss-Hill Average of the Two Approximation of Bulk Modulus, Young Modulus and Poisson Ratio.

Materials	Bulk Modulus	Young Modulus	Shear Modulus	PoissonRatio	B/G
Fe ₃ Al	228.642671	218.41607	81.808653	0.33569	2.7948

The shear elastic deformation which depends on the ratio (B/G) is a parameter that could be used to detect a favorable thermoelectric material [Hong, et al., 2016], the smaller the value, the favorable the materials are for application.

Our calculated value of of B/G is 2.7948 and 1.7231, which shows that Fe₃Al have high resistance which complies to shear deformation and good machinability because it is greater than the value (1.06). Furthermore, our calculated elastic constants (C_{11} , C_{12} and C_{44}) satisfied the following machinability condition for cubic structure: $C_{11}-C_{12}> 0$, $C_{44}> 0$ and $C_{11} + 2C_{12}> 0$. The empirical relationship between bulk and shear moduli (B/G) as proposed Pugh, (Pugh, 1954) could be used to describe the mechanical strength of materials. He suggested that if the B/G ratio is less than 1.75, the material is brittle in nature otherwise, it is ductile. Relying on this assumptions, we found that the B/G ratio for Fe₃Al is 2.7948 , that is to say that Fe₃Al is ductile and AlAs is brittle.

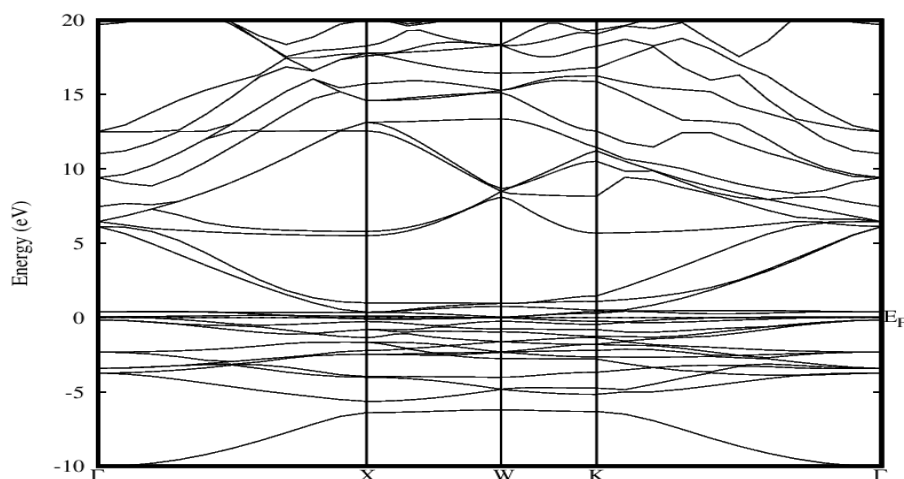
4.4 Electronic Properties

For better understanding of the bonding characteristics and to exploit the underlying

structural stability and elastic properties, we calculated and discussed the band structure within spin polarized approach are presented in the figure below for energy range [-10; +5]eV, with respect to the Fermi level which is chosen to be zero. The band structure has been plotted along the high symmetry points of the cubic Brillouin zone.

The system exhibits a low density of states around the Fermi level, contrary to the k-phase. We have analyzed the electronic levels in terms of atomic orbital decomposition. Around [-10; -5] eV the states of aluminium hybridized slightly with the s state of iron, while around the Fermi level [-5; 0] eV the p Al states hybridize with the d-Fe states.

The electronic band structure for calculations for Fe₃Al were done using pseudo potential and plane wave basis set method within the density functional theory (DFT), treating exchange-correlation functional with generalized gradient approximation(GGA) in the form of Predew Berke-Erzndof (PBE) functional as implemented in Quantum Espresso package.

**Fig. 4. Electronic band structure of Fe₃Al**

4.5 Thermodynamic Properties

The thermodynamic properties results for Fe₃Al is presented in the figure below and its discussion follows: The Fig. 7 is a plot of Debye vibrational energy against temperature which shows that at low temperature the debye vibrational energy is constant, but as the temperature increases rapidly the debye vibrational energy increases correspondingly. Furthermore, the thermodynamic properties entails the specific heat capacity at constant

temperature and entropy. Also, as the debye vibrational free energy decreases the temperature increases. In the Fig. 7, the debye model correctly predicts the low temperature dependence of heat capacity, which is proportional to the debye T³ law. Just like the Einstein model, it also recovers the Dulong-Petit law at high temperatures. But due to simplifying assumptions, its accuracy suffers at intermediate temperatures. At room temperature debye specific heat (C_v) is 70 (J/K/Nmol).

Table 4. The specific heat capacity (C_v), Debye Temperature (θ_D) and the sound velocity of Fe₃Al

Compound	Specific heat(C _v)	Debye temperature(K)	Sound Velocity(m/s)
Fe ₃ Al	90.10709739	438.416	3281.794

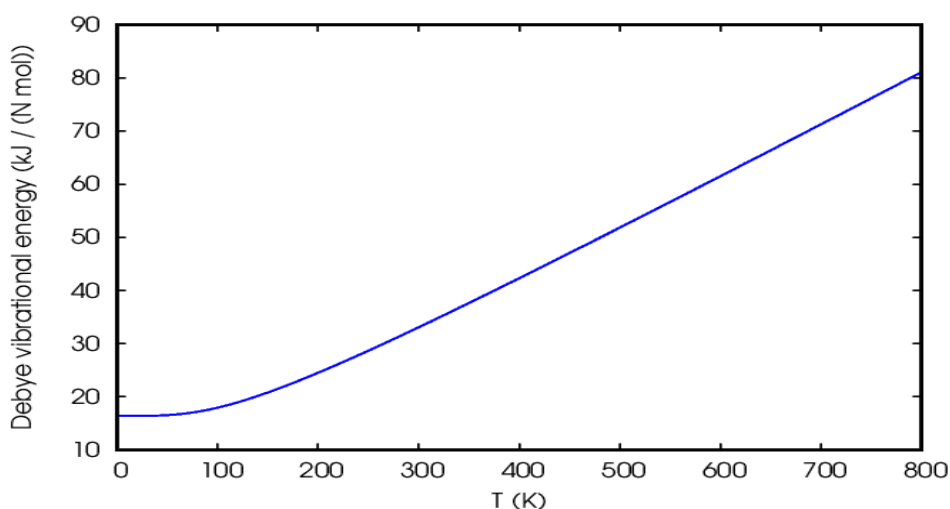


Fig. 5. Debye Vibrational Energy (KJ/Nmol) against Temperature (K) for Fe₃Al

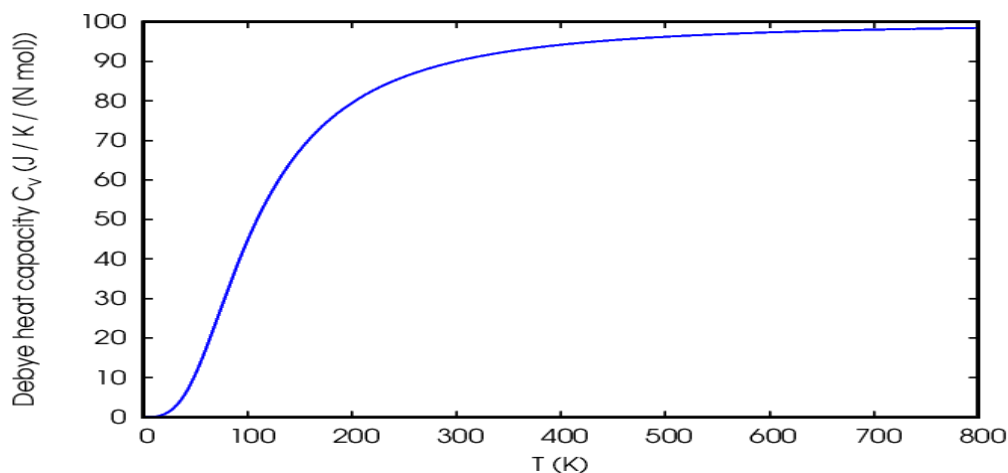


Fig. 6. Specific Heat Capacity of Fe₃Al in the temperature range of 0-800K

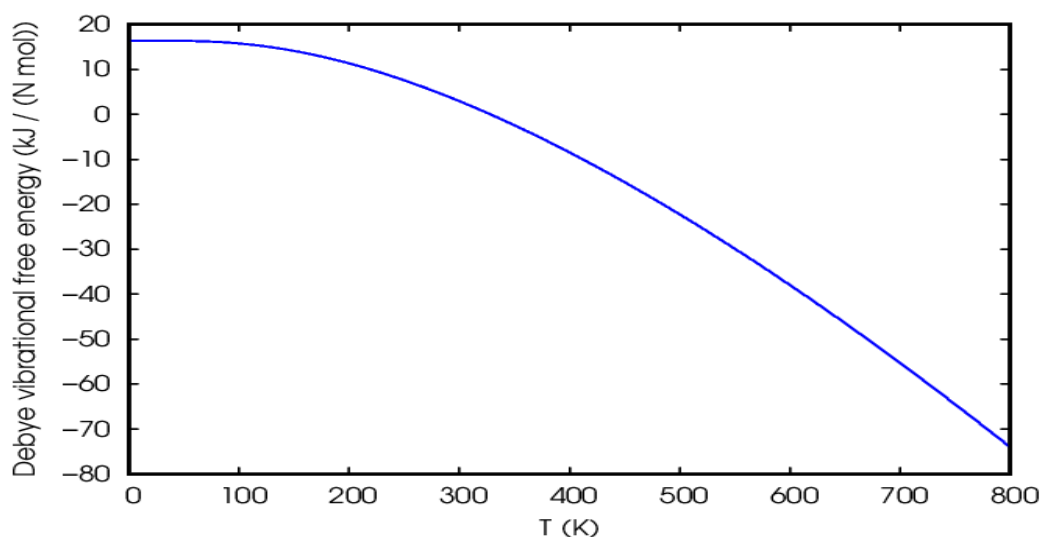


Fig. 7. Debye Free Energy of Fe₃Al in temperature of 0-800K

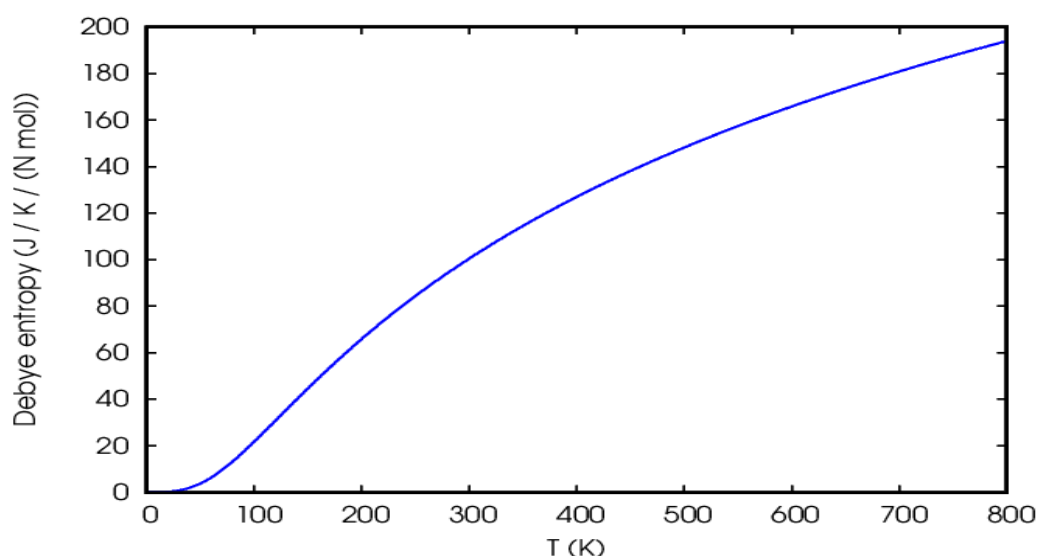


Fig. 8. The entropy of Fe₃Al in the temperature range of 0-800K.

5. CONCLUSION

The Structural, Electronic, Mechanical and Thermodynamic properties of Fe₃Al were determined.

The lattice constant was calculated to be 5.31 a.u, the mechanical stability conditions on the elastic constants in cubic crystals, i.e., $C_{11}-C_{12} > 0$, $C_{11} + 2C_{12} > 0$, are well satisfied for Fe₃Al structure. The ratio of bulk modulus to shear of Fe₃Al is 2.7 which indicates a ductile material. The thermal parameters; sound velocity, debye temperature and heat capacity were calculated for Fe₃Al as given in Table 4.

The first principle calculation was employed using Quantum Espresso program and it was successfully carried out in determining the Structural, Mechanical, Thermodynamic and Electronic properties of Fe₃Al alloys. Also from the result gotten, we observed that the valence and conduction bands overlap considerably for intermetallic compounds in general and there is no band gap at Fermi level. This findings confirm the metallicity of the compound.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Sauthoff G. State of intermetallics development. *Mater. Corros. Und Korros.* 47 1996 through Fe + Al elemental route. *Mater. Sci. Eng*; 2002.
2. Stoloff NS, Iron Aluminides: present status and future prospects, *Mater. Sci. Eng., A* 1998;258.
3. Eggersmann M, MehrerH. Diffusion in intermetallic phases, Diffusion in intermetallics phase of the Fe-Al system. *Philos. Mag*; 2000.
4. Tortorelli PF, NatesnK. Critical factors affecting the high-temperature corrosion performance of iron aluminides. *Mater. Sci. Eng.*1998;A 258.
5. Natesan K. Corrosion performance of iron aluminides in mixed-oxidant environments. *Mater. Sci. Eng.*; 1998.
6. Deevi SC, SwindemanRW. Yielding, hardening and creep behavior of iron aluminides. *Mater. Sci. Eng.*1998;A 258.
7. Deevi SC, SikkaVK. Nickel and Iron aluminides: An overview on properties processing, and applications. *Intermetallics*.1996;4.
8. Hajaligol MR, DeeviSC, SikkaVK, ScoreyCR. A thermomechanical process to make iron aluminide FeAl sheet. *Mater. Sci. Eng.*1998;A 258.
9. Munir ZA, Anselmi-TamburiniU. Self-propagating exothermic reactions: The synthesis of high-temperature materials by combustion, *Mater. Sci. Rep.* 1989; 3.
10. Mossino P. Some aspects in self-propagating high-temperature synthesis, *Ceram. Int.* 2004;30.
11. Rabin BH, WrightRN. Synthesis of iron aluminides from elemental powders: Reaction mechanisms and densification behavior. *Mentall. Trans.* 1991;A 22.
12. Godlewska E, SzczepanikS, ManiaR, KrawiarzJ, KozinskiS. FeAl materials from intermetallic powders. *Intermetallic*.2003;11.
13. Gao H, HeY, ShenP, ZouJ, XuN, JiangY, et al. Porous FeAl intermetallics fabricated by elemental powder reactive synthesis. *Intermetallics*.2009;17.
14. Kang HZ, HuCT. Swelling behavior in reactive sintering of Fe-Al mixtures. *Mater. Chem. Phys.* 2004;88.
15. Poshec E, JozwiakS, KarczewskiK, BojarZ. Fe-Al phase formation around SHS reactions under isothermal conditions. *J. Alloys Comp.* 2011;509.
16. Sina H, Corneliusson J, Turba K, Iyengar S. A study on the formation of iron aluminide (FeAl) from elemental powders. *Journal of Alloys and Compounds.* 2015 Jul 5;636:261-9.
17. Wang X, WoodJV, SuiY, LuH. Formation of intermetallic compounds in iron aluminium alloys. *J. Shanghai Univ. English Ed.* 1998;2.
18. Shahverdi HR, GhomaschiMR, ShabestariS, HejaziJ. Microstructural analysis of interfacial reaction between molten aluminum and solid iron. *J. Mater Process. Technol.*2002;124.

© 2021 Okunzuwa and Eddy; This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Peer-review history:

The peer review history for this paper can be accessed here:
<http://www.sdiarticle4.com/review-history/67620>