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Structural and Electronic Properties of $FeNi_3$ and $FeNi_2Pt$ Alloys

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The ab initio pseudopotential method is based on Density Functional Theory (DFT), in which the Generalized Gradient Approximation (GGA) according to the scheme described by Perdew-Burke-Ernzerhof (PBE) is used. The method is implemented using Siesta software to investigate the structural, electronic and magnetic properties of the fcc phase of $FeNi_3$ and $FeNi_2Pt$ alloys. In fact, it is a useful and effective program, and it can be considered a good method for predicting the crystal structure and its properties, which has been confirmed. The structure was subjected to a relaxation process in order to search for the structural parameters, and the results obtained are consistent with the available experimental and theoretical data. So, these results can be considered a good expectation, indeed, the calculated structural parameters for this compound are in agreement with the available experimental data. The lattice constants and band gaps at a pressure value of zero are found to be consistent with the previous work. The results of the band structure calculated by GGA for the $FeNi_3$ alloy are compared with those obtained for the $FeNi_2Pt$ alloy, where it was found that the valence band levels are very close to each other in $FeNi_3$ alloy compared to $FeNi_2Pt$ alloy. The total density of states (TDOS) shows the process of electron density distribution in the region close to the Fermi level for both compounds. The partial density of states (PDOS) shows most of the effect of the distribution of 3*d* states in the electron distribution of the two alloys, and the $FeNi_2Pt$ alloy shows more ferromagnetism than the $FeNi_3$ alloy.

Keywords: DFT, $FeNi_3$ alloy, $FeNi_2Pt$ alloy, Energy formation, Band structure, Density of states (DOS).

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1. INTRODUCTION

Studies on Fe-Ni systems and, in particular, $FeNi_3$, are among the studies that have long and widely occupied the minds of researchers [1, 2]. These systems also have several wide uses, as they are used in many advanced sensitive applications, due to their high magnetic permeability, low strength, magnetic stenosis close to zero, and they also have variable magnetic resistance, depending on the surrounding conditions. On the other hand, if we want to shed light on its other properties, for example mechanical properties, we find that $FeNi_3$ is an alloy with low strength and corrosion resistance at the same time, which qualifies it to be among the wide uses and in various fields.

Iron-nickel alloys, as traditional soft magnetic materials, have received great attention due to their high saturation (MS) magnetization, high permeability, and high Curie temperature, while their energy losses are in a low form. With its features, it has been widely used in absorbing electromagnetic waves. magnetic sensors, magnetic recording heads, and even pharmaceuticals [3]. Fe-Ni alloys have attracted researchers because of their excellent thermal, magnetic and optical properties [4]. Numerous experimental research studies have been conducted on both iron and nickel alloys. Recently, the structural constants, elastic, electronic and magnetic properties of three Fe-Ni binary metals ($FeNi_3$, FeNi and Fe_3Ni) under pressure change were studied by M.J wang et al. [5] using first principle DFT.

In this work, we will study the $FeNi_3$ alloy from the structural and electronic properties on the one hand, and on the other hand, we will doped the $FeNi_3$ alloy with platinum metal, where we replace the nickel Ni atom with the platinum Pt atom, to study the $FeNi_2Pt$ alloy again and highlight its new properties and compare it with the alloy in its normal state This work will be based on the use of density function theory.

2. COMPUTATIONAL DETAILS

In this work, we have based our calculations on the principles of sigmoid-polarized density functional theory (DFT) [6, 7]. In terms of exchange and correlation functional, the Generalized Gradient Approximation (GGA) functional was applied according to the suggestions of Perdew, Burke and Ernzerhof (PBE) [8]. The process of structural relaxation of the ingot has been studied by simulating the first density functional principle. which is descended in the atomic-orbital numerical method according to the implementation of the SIESTA code [9, 10]. The alloys structures were also confirmed using the MATERIAL STUDIO program code [11]. Extended wave functions took place in plane-wave basic groups using a kinetic energy cutoff of 400 eV. This was applied to all systems included in our research. Monkhorst- Pack grid having special *k*-point meshes was used to carry out the integrations of Brillouin zone. In terms of implementing self-consistent field calculations, the convergence criterion of 10^{-4} on to the total energy was used for this purpose. While we suggested that the value of maximum tolerance for the displacement of ions in the block is 0.05 Å. The arrays in the output of the Q-Chem program provided the

optimal electronic structure for each alloy. The electronic and optical properties were calculated based on both total electronic energy and self-consistent field (SCF) orbital energy values.

3. RESULTS AND DISCUSSION

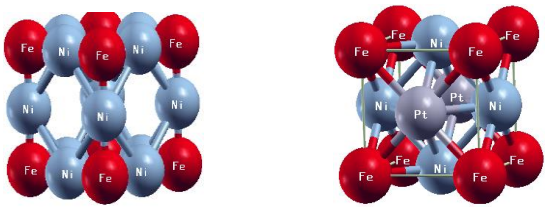
3.1 Primary Cell Structure

The lattice constants of $FeNi_3$ and $FeNi_2Pt$ alloys have been investigated many times over several decades. The stable primary cell structure of $FeNi_3$ is cubic fcc characterized by the Pm3m group and lattice constants estimated as $a = b = c = 3.528$ Å, $\alpha = \beta = \gamma = 90.00°$. $FeNi_3$ and $FeNi_2Pt$, crystallize in the most stable form in a cubic structure, as shown in Fig. 1.

Each $FeNi_3$ consists of four atoms, one Fe atom occupying the (0, 0, 0) and three Ni atoms occupying the following (1/2, 1/2, 0), (1/2, 0, 1/2), (0, 1/2, 1/2) positions. The calculations in this study are based on the Siesta software that was used to calculate the initial cell constants for $FeNi_3$. The alloy was also doped with a platinum Pt atom at position (1/2, 1/2, 0) to obtain the $FeNi_2Pt$ alloy. The results are given in Table 1.

Table 1 – Comparison of the primary cell constants of $FeNi_3$ and $FeNi_2Pt$ with theoretical and practical results

Alloy	Ref.	a (Å)	b (Å)	c (Å)	V (Å)	E_F (eV)
$FeNi_3$	Our work	3.528	3.528	3.528	43.88	– 4.784
	Theory [12]	3.548	3.548	3.548	44.662	
	Theory [13]	3.50	3.50	3.50	/	
	Exp [13]	3.55	3.55	3.55	/	
FNi_2Pt	Our work	3.563	3.563	3.563	45.30	– 2.496



a b

Fig. 1 – Structure of $FeNi_3$ (a) and $FeNi_2Pt$ (b)

Using DFT and the Siesta program, we were able to calculate the primary cell constants, and then using the GGA to find the values 3.528 Å for the constant a, b and c this is for the $FeNi_3$ alloy and value 3.563 Å for the constant a, b and c for the $FeNi_2Pt$ alloy. It is noted that these results are in agreement to a large extent with the theoretical and experimental results [13, 14] shown in Table 1.

In addition, we calculated the percentage error in the obtained values. Assuming it is compared with the experimental values taken as reference, we find that the error value has been estimated to be 0.8 % for the constant a, b and c with the approximation to GGA. Accordingly, the calculated error values are very small, which shows that the method adopted in the calculation is logical and reasonable. The doping process showed its effect in changing the structure of the primary cell, causing an increase in the bond length between the iron and nickel atoms, which also resulted in an increase in the cell size compared to the cell in the normal state.

3.2 Formation Energy

The formation energy of $FeNi_3$ and $FeNi_2Pt$ was calculated using the following relationship:

$$E_C = E_T[\mathrm{FeNi_3}] - E_T[\mathrm{Fe}] - E_T[\mathrm{Ni}] - E_T[\mathrm{Pt}], \quad (1)$$

where E_T[$FeNi_3$] is the total energy of $FeNi_3$ and $FeNi_2Pt$ in the solid state, E_T[Fe] is the total energy of the free Fe atom, E_T[Ni] is the total energy of the free Ni atom, E_T[Pt] is the total energy of the free Pt atom, Ec is the formation energy.

The results of calculating the formation energy of $FeNi_3$ and $FeNi_2Pt$ are shown in Table 2.

Table 2 – Formation energy of $FeNi_3$ and $FeNi_2Pt$ alloys

Alloy	Formation energy (eV)
$FeNi_3$	– 18.0065
$FeNi_2Pt$	– 13.487

The obtained value of $FeNi_3$ formation energy was – 18.0065 eV and for $FeNi_2Pt$ was – 13.487 eV. These results indicate that $FeNi_3$ alloy is the most stable compared to $FeNi_2Pt$ alloy, and this is logical, as the compound in its normal state is more stable than in the case of doped with any other metal.

3.3 Electronic Properties

3.3.1 Structure of Energy Bands

In order to study the basic structure of the structure, we choose a region called Brillouin in order to find the electronic properties of the material. Fig. 1 shows the Brillouin region related to the cubic. It is worth noting that the study of properties on this region can be generalized later to $FeNi_3$.

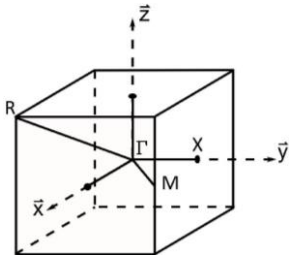


Fig. 2 – Brillouin region of a cubic crystal

We used the DFT theory and GGA approximation to determine the band gap of $FeNi_3$ and $FeNi_2Pt$. This method has been relied upon because it is one of the most appropriate methods for studying the electronic structures of materials. The energy band structure of $FeNi_3$ and $FeNi_2Pt$ alloys was calculated for the above obtained lattice constants ($a = b = c = 3.528$ Å, $\alpha = \beta = \gamma = 90.00°$). The structure of energy bands of alloys is shown in Fig. 2.

It is noticeable in Fig. 2a and 2b, which the highest valence bands overlaps with the conduction bands, and this is evidence of the metallic property of the two alloys. Each of the two alloys has ferromagnetic properties, as the magnetic moments are estimated at values 5.071 μB 5.20 μB for $FeNi_3$ and $FeNi_2Pt$, respectively.

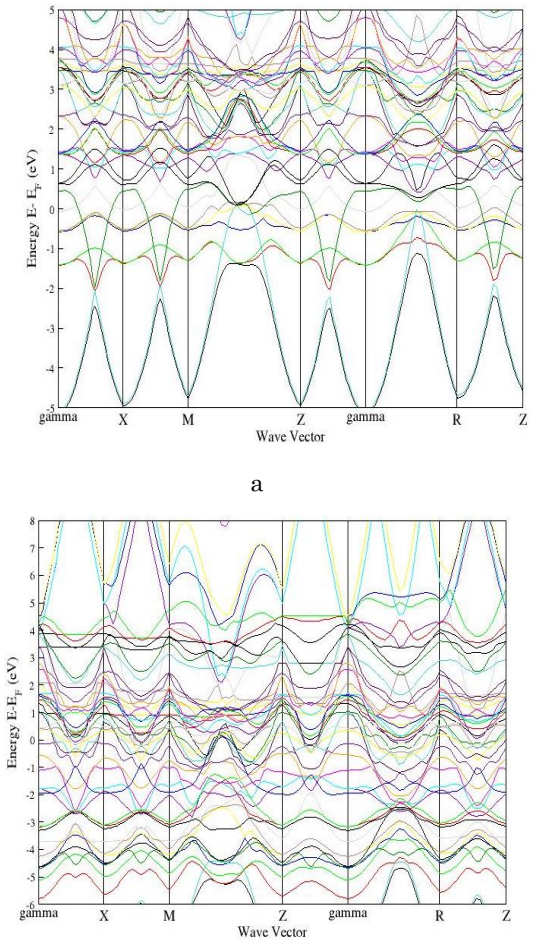


Fig. 3 – Energy band structure of (a) $FeNi_3$, (b) $FeNi_2Pt$

3.3.2 Electronic Density of States (DOS)

We analyze the total density of states (TDOS) and partial density of states (PDOS) for $FeNi_3$ and $FeNi_2Pt$ alloys using the GGA approximation so as to determine the reason for the presence of states that formed the valence and conduction bands and to understand the nature of the interactions between the atoms of the two studied alloys, as shown in Fig. 4 and Fig. 5, respectively.

Fig. 4a and Fig. 4b show that the calculated TDOS for $FeNi_3$ and $FeNi_2Pt$ have high values with GGA Approximation in the region close to the Fermi level and the TDOS value of $FeNi_2Pt$ is higher than $FeNi_3$ this means that the valence band is rich in electrons. Close to the Fermi level, we find that the highest peak of the density of states was recorded at the $FeNi_2Pt$ alloy, which was estimated at 5.35 eV/states), while the value 4.08 eV/states was recorded as the highest value for $FeNi_3$ alloy. In both Fig. 4a and Fig. 4b, the number of states with spin in the energetically region from – 5 eV to Fermi level in DOS (right part), corresponding to the occupied, (i.e., electron-like), subbands in the band structure (left part), is dramatically overwhelming that for spin, making $FeNi_3$ and $FeNi_2Pt$ good soft-ferromagnetic material.

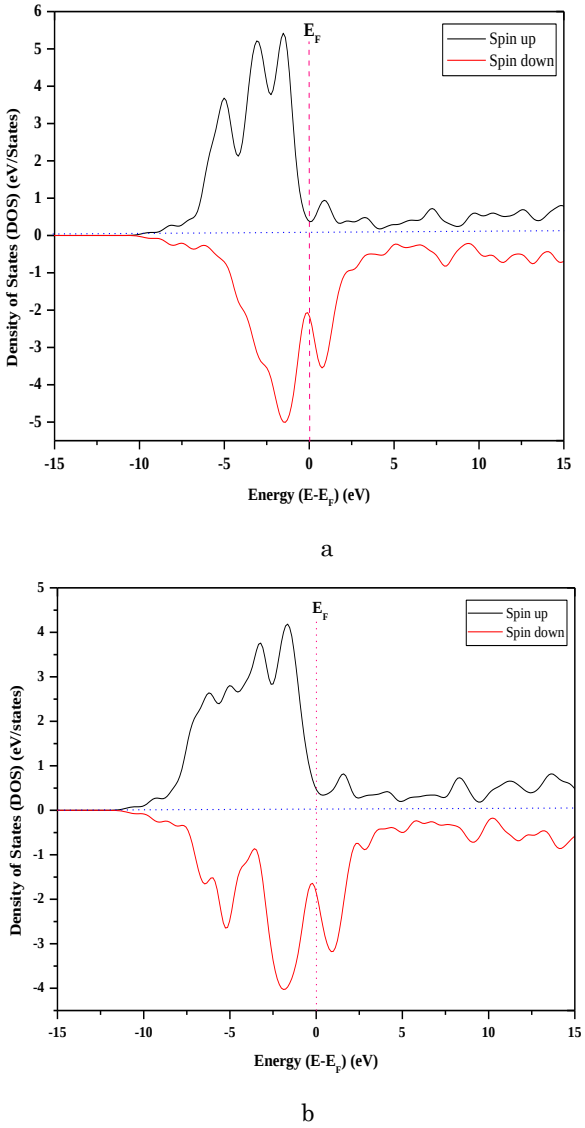
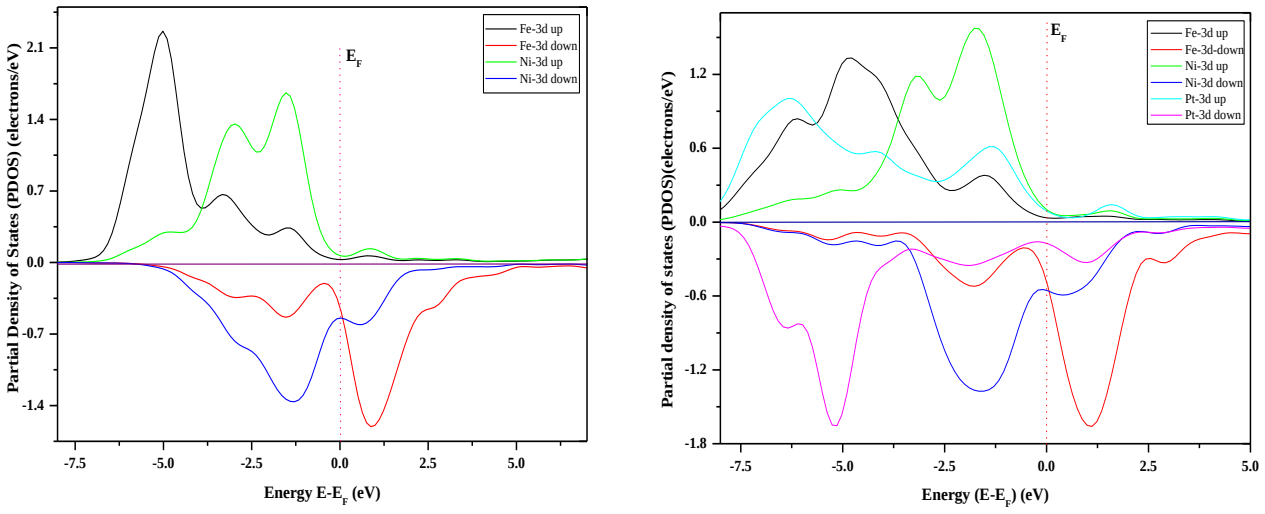


Fig. 4 – Total density of states (TDOS) for :(a) $FeNi_3$ and (b) $FeNi_2Pt$

3.3.3 Partial Density of States (PDOS)

In this study, the partial density of states (PDOS) of $FeNi_3$ and $FeNi_2Pt$ alloys is calculated and annotated in detail to understand the movement of electrons close to the Fermi level. Fig. 5a and Fig. 5b show PDOS for $FeNi_3$ and $FeNi_2Pt$ respectively with GGA approximation.

We represent the density of incident states on atomic valence orbitals (PDOS) in order to compare them to reveal the role of electrons in different atomic valence orbitals, and their effect on electronic properties, especially on polarization. Based on the different distributions of spin states (spin up and spin down) represented in the figure, the spin polarization is determined, starting with a single primitive cell and later generalizing to each of the atomic domains. In order to investigate more deeply the contributions of the Fe and Ni atoms constituting the $FeNi_3$ and $FeNi_2Pt$ alloys, we calculated the expected density of states over electron orbitals as a function of energy, $(E - E_F)$.



a b

Fig. 5 – Partial density of states (PDOS) for (a) $FeNi_3$, (b) $FeNi_2Pt$

From the PDOS distributions, shown in Fig. 5a for $FeNi_3$ alloy, it can be shown that the electronic states are mainly located in the active region extending from – 6.5 eV to + 3.5 eV around the Fermi levels. To give more detail, near the Fermi level, Ni atoms have larger 3*d*-orbital states than the Fe atom, has, and a larger port comes from Ni 3*d*-electrons with spin up than those in the same 3*d*-ones with spin down, Also, the contribution of the 3*d* station is dominant in the electronic distribution of the $FeNi_3$ alloy.

As for the $FeNi_2Pt$ alloy, we note a significant contribution of the 3*d* orbital of the platinum Pt atom, which thanks to this contribution provided $FeNi_2Pt$ alloy with a greater probability of electrons being near the Fermi level, which makes this alloy is more ferromagnetic.

4. CONCLUSIONS

The aim of the work was to compare the structural and electronic properties of both $FeNi_3$ and $FeNi_2Pt$ alloys and bring them closer to the available results, using DFT with the help of GGA. We found that the values of the lattice constants are close to the previous theoretical and experimental results, from the band structures, it is indicated that the alloys are conductors. Alloys with an electron density close to the Fermi level are considered to be the best qualified for chemical and thermal activity. We also found that $FeNi_2Pt$ is the best in terms of ferromagnetic property.

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Структурні та електронні властивості сплавів $FeNi_3$ та $FeNi_2Pt$

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Ab initio метод псевдопотенціалу базується на теорії функціоналу густини (DFT), в якій використовується узагальнене градієнтне наближення (GGA) за схемою, описаною Perdew-Burke-Ernzerhof (PBE). Метод реалізовано за допомогою програмного забезпечення Siesta для дослідження структурних, електронних і магнітних властивостей ГЦК фази сплавів $FeNi_3$ і $FeNi_2Pt$. Це дійсно корисна та ефективна програма, і її можна вважати хорошим методом прогнозування кристалічної структури та її властивостей, що і було підтверджено. Структура піддавалась процесу релаксації з метою розрахунку структурних параметрів. Отримані результати узгоджуються з наявними експериментальними та теоретичними даними. Установлено, що сталі ґратки та заборонена зона при нульовому значенні тиску узгоджуються з попередньою роботою. Результати зонної структури, розраховані з використанням GGA для сплаву $FeNi_3$, порівнювались з результатами, отриманими для сплаву $FeNi_2Pt$, де було виявлено, що рівні валентної зони дуже близькі один до одного в сплаві $FeNi_3$ порівняно зі сплавом $FeNi_2Pt$. Сумарна густина станів (TDOS) показує процес розподілу електронної густини в області, близькій до рівня Фермі, для обох сполук. Часткова густина станів (PDOS) демонструє більшу частину ефекту розподілу 3*d*-станів електронів двох сплавів, а в сплаві $FeNi_2Pt$ спостерігаються більші феромагнітні властивості, ніж в сплаві $FeNi_3$.

Ключові слова: DFT, Сплав $FeNi_3$, Сплав $FeNi_2Pt$, Формування енергії, Зонна структура, Густина станів (DOS).