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Comparison of the Optical Properties of Pure and Doped Iron-Nickel Alloys

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The pseudo ab initio ability is based on density function theory (DFT), use of generalized gradient approximation (GGA). In this work we use the Siesta code for the first time in studying this specific $FeNi_3$ and $FeNi_2Pt$ alloys and its fcc phase which enabled us to find the structural and optical properties of $FeNi_3$ and $FeNi_2Pt$ alloys in its fcc cubic crystal structure. Obtained results showed that the structural properties of the cubic phase structure have lattice constants very close to what was previously found in theoretical and experimental studies, and all the optical properties calculated such as absorption coefficient, reflectivity, refractive index, and the imaginary part of the dielectric constant, show that the $FeNi_3$ and $FeNi_2Pt$ alloys They are two electrical conductors, whose valence band is completely overlapped with the conduction band. Through the optical results, it was found that we can use them in the infrared and visible region applications, and this type of work was studied in this research for the first time.

Keywords: Density function theory; $FeNi_3$; Doped; Absorption coefficient; Optical conductivity; Imaginary part

1 Introduction

Among the systems that have long attracted the attention of researchers are Fe-Ni systems, specifically, $FeNi_3$ over several eras[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 delve into 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 materials with wide uses.

Iron-nickel alloys have drawn the attention of researchers because of their excellent thermal, magnetic and optical properties[3]. Numerous experimental research studies have been conducted on both iron and nickel alloys, using neutron and Mossauer experiments, as well as X-ray diffraction[4-6]. The lattice dynamic, thermodynamic and magnetic properties of some of them have been studied for different important phases of the Fe-Ni alloy such as L12 $FeNi_3$, taenite L10 FeNi and L12Fe_3Ni using the density functional theory method[7].

Iron-nickel (Fe-Ni) alloys are of great importance in many industrial and scientific fields. The importance of these alloys, their unique aspects, and the novelty of their study can be summarized as follows:

Superior magnetic properties: Fe-Ni alloys are known for their high magnetic properties, making them ideal for use in applications that require permanent or temporary magnets, such as electric motors and magnetic sensors.

Corrosion and rust resistance: It has high resistance to corrosion and rust, which increases its lifespan and makes it suitable for use in harsh environments[8,9].

As for its excellent mechanical properties: hardness and durability, which makes it suitable for use in the aviation and space industry and heavy engineering structures.

The novelty of current research is the development of new Fe-Ni alloys, by adding other elements to improve physical and chemical properties, such as improving electrical conductivity or increasing corrosion

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resistance, as significant improvements in magnetic and mechanical properties are achieved when the size of crystalline grains is reduced to nano. Which was the focus of our research.

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 dope the $FeNi_3$ alloy with platinum metal. We replace the Ni atom of nickel with the platinum atom of Pt, to study the $FeNi_2Pt$ alloy again and highlight its new properties. We also compare it with the alloy in its natural state. This work will depend on the use of the theory of the density function. This type of study has been studied for the first time in this theoretical form and with a program Siesta.

2 Theoretical Method of Calculation

In this research, We established the calculations on the principles of spin-polarized density-functional theory (DFT)[10]. In terms of exchange and correlation functional, the Generalized Gradient Approximation (GGA) functional was applied according to the sugges-tions of Perdew, Burke and Ernzerhof (PBE)[11]. The main reason for using DFT is to reduce computational complexity. Compared to traditional methods such as the Hartree-Fock method and Post-Hartree-Fock methods, DFT is more computationally efficient and allows larger systems to be studied with fewer computational resources. DFT can also be used to study systems containing hundreds to thousands of atoms, making it ideal for studying solids, surfaces, and nanomaterials. The Generalized Gradient Approximation (GGA) function is an important development to improve the accuracy of calculations compared to simpler approximations such as the Local Density Approximation(LDA), GGA is successfully used to study solids, surfaces, molecules, and nanomaterials, improving geometric predictions and electronic properties, Results calculated using GGA are often closer to experimental values, which enhances the reliability of theoretical models.

The increase in geometries of clusters was made through functional density first principle-simulations technique, which is rooted in the numerical atomic orbital method according to SIESTA code implementation[12]. SIESTA (short for Spanish Initiative for Electronic Simulations with Thousands of Atoms) is an open-source software package used to perform molecular dynamics simulations, structural calculations of solids and molecules based on density functional theory (DFT). The software was developed to be able to process systems containing thousands of atoms with high efficiency thanks to the use of advanced computational methods. SIESTA can handle very large systems *e.g*. $FeNi_3$ and $FeNi_2Pt$ alloys, while reducing the time required for calculations. It can study the electronic, structural, optical, dynamic, and thermal properties of solids and molecules. 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. Actually, 0.05 Å was the value of the maximum tolerance for ion displacement in the cluster. We obtained the optimized structures when the atomic forces were less than 0.005 eV/Å. Z-matrices in the Q-Chem program output, which provided the optimized electronic structure for each cluster. However, we calculated electronic properties based on both self-consistent field (SCF) total electronic energy and orbital energy values.

3 Results and Discussion

3.1. Stable Structure of Alloys

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.

Using DFT and the Siesta program, we were able to calculate the primary cell constants. By employing the GGA,we obtained values of 3.528 Å for the constant a, b and c this is for the FeNi3 alloy and value 3.563 Å for the constant a, b and c for the $FeNi_2Pt$ alloy. Notably, that these results are in

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

alloy	work	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 [13]	3.548	3.548	3.548	44.662	
	Theory [14]	3.50	3.50	3.50	/	
	Exp [14]	3.55	3.55	3.55	/	
FNi_2Pt	Our work	3.563	3.563	3.563	45.30	-2.496

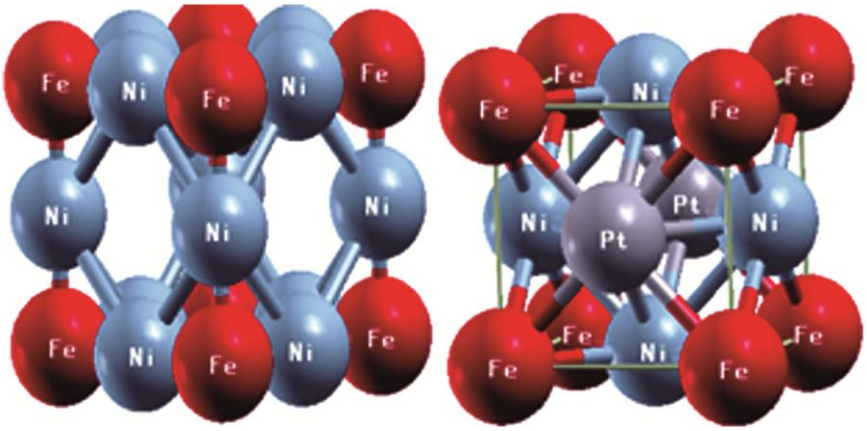

Fig. 1 — Structure : (a) $FeNi_3$, (b) $FeNi_2Pt$ alloys

substantial agreement to a large extent with the theoretical and experimental results[13,14] shown in Table 1.

In order to study the basic structure of the material, we chose a region called Brillouin in order to find the electronic properties of the material in that region and then generalize the properties to the rest of the matter. Fig. 1 shows the Brillouin region of a cube. It is noteworthy that the study of properties in this region can be generalized later to $FeNi_3$ and $FeNi_2Pt$ alloys.

We used 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, α = β=γ= 90.00°. The structure of energy bands of alloys is shown in Fig. 2.

The Brillouin zone holds significant importance in the fields of solid-state physics and materials science, as it encompasses the wave vectors characteristic of the crystal system within reciprocal space. Its shape and size are determined by the specific crystal lattice and its geometric structure. By comprehending the Brillouin zone and its properties, we gain valuable knowledge about the electronic structure, phonon dispersion, and other fundamental characteristics of crystalline materials. This understanding plays a crucial role in analyzing the behavior of electrons and phonons in solids, ultimately contributing to the development and application of novel materials in various technological fields.

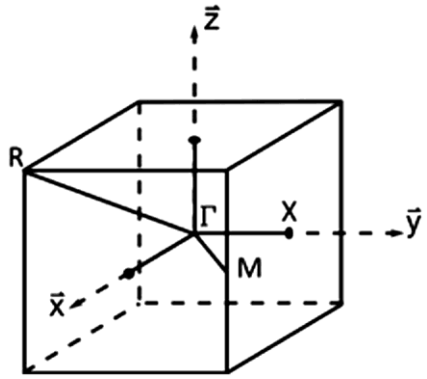

Fig. 2 — Brillouin region of a cubic crystal

3.2. Optical Properties

The study of the optical properties of materials is of great importance for obtaining the required information about the values of the optical constants of the material over a wide range of wavelengths. Based on this information, these materials can be used for manufacturing optical pieces and optical pulses with different uses.

3.2.1. Absorption Coefficient

It is the decreasing ratio in the intensity of the spectrum of incident radiation energies with respect to

the unit distance in the direction of wave propagation within the medium. The absorption coefficient can depend on the energy of the incident photons and the properties of the conductors. The nature of electronic transitions can be known through the values of the absorption coefficient, its equation in the form:

$$\alpha = \frac{4\pi K}{\lambda} \quad \ldots (1)$$

Where α is absorption coefficient, k is the coefficient of extinction and λ is wave length (cm).

The adsorption coefficient values for $FeNi_3$ and $FeNi_2Pt$ alloys were calculated with approximations of GGA, and they are shown in Fig. 3.

Figure 3 shows the change in the absorption coefficient as a function of the energy of the incident photon on the $FeNi_3$ and $FeNi_2Pt$. It is clear from the general figure that the absorption coefficient of the two alloys has oscillating values between increasing at times and decreasing at other times. The values of the absorption coefficient begin to increase rapidly with the increase in the energy of the photons of light until the amount of energy 1.1 eV, with respect to $FeNi_3$ and energy 1eV with respect to $FeNi_2Pt$. We also notice the absence of an absorption threshold as found in semi-conductors; these alloys are not transparent at all. We record the highest value of the absorption coefficient for $FeNi_3$ alloy at energy 6 eV, while we record the highest value of the modulus of the $FeNi_2Pt$ alloy in the energy limits 3.7 eV. This indicates that the change in the energy of the incident photons leads to different optical behaviors in this material. This result is close to work[15].

3.2.2. Optical Conductivity

It is a physical property that binds the current density to the general frequency electric field and that is closely related to the dielectric constant known as the following equation:

$$\sigma(\omega) = \frac{J(\omega)}{E(\omega)} \quad \ldots (2)$$

Where σ is optical conductivity (Sm/m), J is current density (A/m^2) and E is electric field (N/C).

The optical conductivity values for alloys were calculated with approximations of GGA, the results are as shown in Fig. 4.

Fig. 4 represents the optical conductivity changes in terms of the energy of photons falling on the alloys using the GGA approximations.

We notice from the figure in general that the optical conductivity curve fluctuates between increase and decrease with increasing energy of the incident photons. It is also noted that the curves of the two alloys are almost identical in values, except for recording higher peaks at energy 0.5 eV and 2.2 eV in the $FeNi_2Pt$ alloy. This is the case within the infrared and visible regions, which suggests that the $FeNi_2Pt$ alloy is the best for optical applications.

3.2.3. Refractive Index

It is the ratio between the speed of light in free space and its speed in the matter, and the refractive index can be found according to the following equation:

$$n_0 = \left[\left(\frac{1+R}{1-R}\right)^2 - (k_0^2+1)\right]^{\frac{1}{2}} + \frac{1+R}{1-R} \quad \ldots (3)$$

The refractive index values for $FeNi_3$ and $FeNi_2Pt$ were calculated using the GGA approximations as shown in Fig. 5.

From Fig. 5, which expresses the refractive index in terms of the incident photons, the value of the static refractive index (n_0) for $FeNi_3$ and $FeNi_2Pt$ alloys are

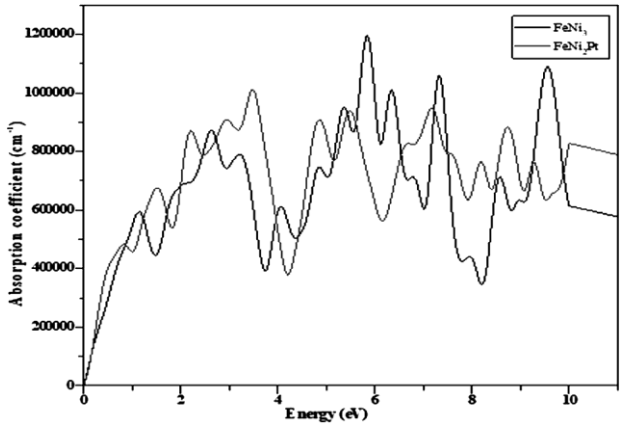

Fig. 3 — Absorption Coefficient of $FeNi_3$ and $FeNi_2Pt$ alloys

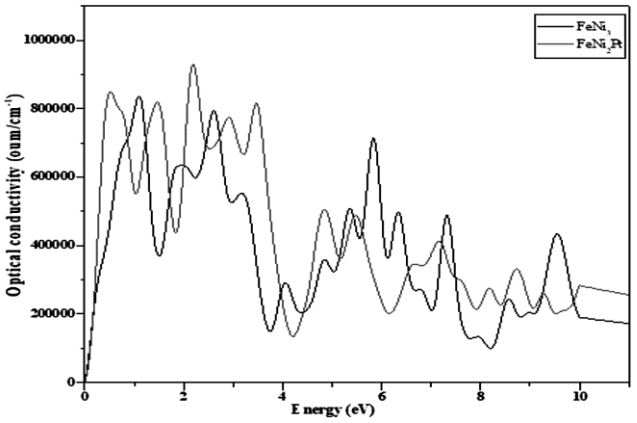

Fig. 4 — Optical Conductivity of $FeNi_3$ and $FeNi_2Pt$ alloys

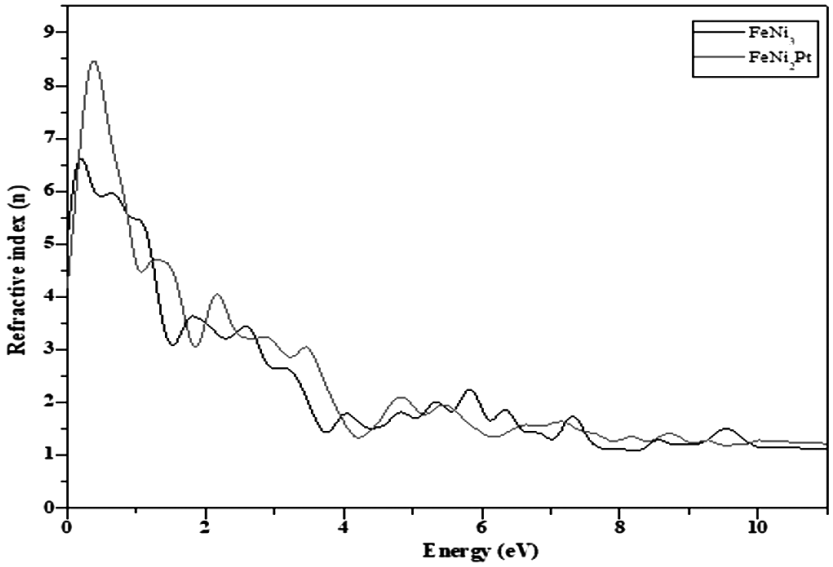

Fig. 5 — Refractive index of $FeNi_3$ and $FeNi_2Pt$ alloys

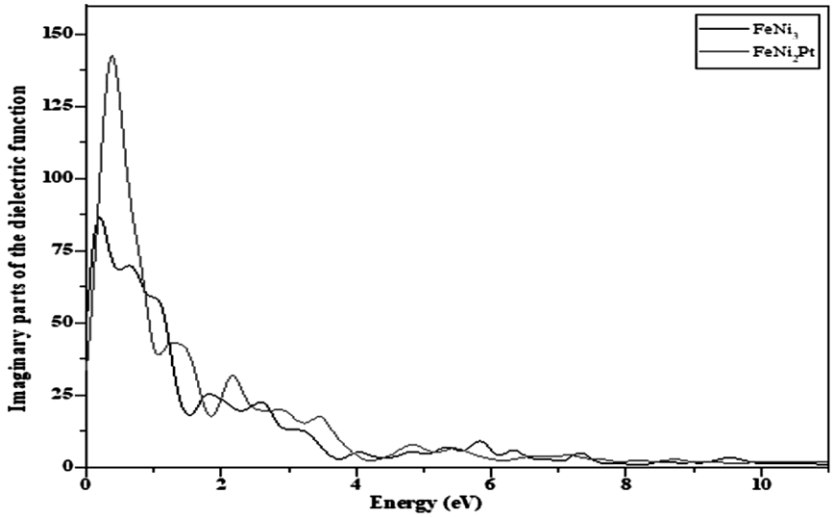

Fig. 6 — The Imaginary Part of the dielectric constant of $FeNi_3$ and $FeNi_2Pt$ alloys

4.5. After that, the refractive index is in-creased until the value becomes 6.5 at an energy value of 0.25 eV for $FeNi_3$, While the value of the refractive index of the $FeNi_2Pt$ alloy rises to the value 8.48 at energy 0.6 eV. The presence of small and decreasing vibrations is recorded to reach the value zero, and this is fully consistent with the work[16].

3.2.4. Dielectric constant

When the interaction between the light and the charges of the medium is the result of the process of absorbing the energy of a substance, the interaction results in the polarization of that medium. This polarization is described by the dielectric constant, which is known by the following relationship:

$$\varepsilon = \varepsilon_r - i\varepsilon_i \quad \ldots (4)$$

Where is complex dielectric constant, is real part of the dielectric constant and is imaginary part of the dielectric constant.

The values of the dielectric constant in its imaginary part for the $FeNi_3$ and $FeNi_2Pt$ were calculated by approximating GGA as presented in Fig. 6.

Figure 6 represents the change of the imaginary part of the dielectric constant (ε_i) using the GGA approximations. To this end, we have observed that the curves of the imaginary part of the dielectric constant of the two alloys are almost identical and that they are in an oscillatory manner, except for what is recorded in the region (0 to 1.2) eV where we notice

large values of the imaginary part of the $FeNi_2Pt$ alloy. In general, this amount indicates that the two alloys are electrical conductors.

The results obtained through this study show how close they are to the results obtained experimentally, and this is demonstrated by the following works[17].

Potential applications based on optical properties of alloys egg, in magnetic lenses: that is, in electron microscopes and laser devices, due to their high magnetic permeability, nickel and iron alloys are used to form magnetic lenses that focus electron beams in electron microscopes or modify the path of light in lasers. In smart windows: The alloys used nickel and titanium (NiTi) alloys with shape memory, where These alloys can change their optical properties in response to changes in temperature, which allows dynamic control of the passage of light in mirrors with low thermal expansion such as telescopes and lasers. It has a very low coefficient of thermal expansion, which makes it ideal for making optical mirrors that maintain their precise shape under temperature changes, thus ensuring high accuracy in telescopes and lasers.

The optical properties of alloys are integral to their applications in modern technology. By tailoring the composition, microstructure, and doping of alloys, researchers and engineers can develop materials with specific optical characteristics suited to a wide range of applications, from medical therapies to advanced optoelectronic devices. Understanding and leveraging these properties is crucial for the ongoing innovation and improvement of technology in various fields.

4 Conclusion

Based on the calculations carried out according to the density function theory (DFT) and the use of the two used Siesta programs, and as a result of comparing the results obtained through the approximation (GGA) of the $FeNi_3$ and $FeNi_2Pt$ alloys, whether structural or optical results, we conclude that:

The structural results indicated that the network constants of the primary cell in the $FeNi_3$ alloy gave results very close to what was reached in previous theoretical and experimental studies. The doping of the cell with a platinum seed affected the increase in its size without changing its shape.

The value of the imaginary part of the dielectric constant confirmed that the two alloys behave like conductors. This was also confirmed by the results which the absorption coefficient, reflectivity and refraction coefficient confirm. In addition to that, the $FeNi_3$ and $FeNi_2Pt$ alloys are good candidates for applications that fall within the visible infrared range. the results of the optical properties calculated for $FeNi_2Pt$ alloy are better than $FeNi_3$ alloy, and this is what makes it likely to be used in optical applications.

As directions for future research, there are two ways to enhance magnetic properties: by increasing magnetic permeability. This is achieved by improving the crystal structure and controlling the ratio of nickel to iron to achieve the best magnetic performance. Another approach is to form alloys with lower thermal expansion .In the field of Nano-alloy, researchers are attempting to use nanotechnologies to improve performance and increase efficiency in optical and magnetic applications such as optoelectronics. This involves exploiting the unique properties of alloys to improve the performance of optical devices such as light-emitting diodes (LEDs) and light detectors.

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