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Research Article

Electronic and Optical Properties of FeNi2Mn and FeNi2Cr Alloys Using the Density Function Theory

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Abstract:

Iron and nickel alloys attract great interest from researchers due to their distinctive properties and thus their use in many technological and practical applications. The structural, electronic and optical properties of the FeNi2Mn and FeNi2Cr alloys were studied using the first-principles planar wave method compatible with the ultra-soft pseudo potential scheme under the density functional theory (DFT). The calculated equilibrium lattice constant for FeNi3 is very close with other available results. It turns out that the large contribution of d electrons in the total electronic density of states is dominant, which in turn affects the electronic and magnetic properties of these alloys. The electronic band structure, total and partial electron density were analyzed and it was concluded that the FeNi2Cr alloy has a greater magnetic, the absorption coefficient, optical conductivity, and refractive index of the two alloys were calculated and analyzed, and based on that, they will be used in the appropriate technological applications.

1. Introduction

Fe-Ni systems, in particular, FeNi (Permaloy criterion), have been studied during the past decades within a wide range [1–3]. It is also used in many advanced applications, as a result of its high magnetic permeability, low strength, and close to zero magnetic stenosis, as well as its magnetic resistance with varying features. Also used in electromagnetic wave absorbers, antennas, magnetic sensors, actuators, magnetic recording heads, and pharmaceuticals [4]. In the event that the molar ratio of Fe to Ni is 1:3, the compound $FeNi_3$ can be formed with a series of distinct properties. The metallic $FeNi_3$ having a space group FCC crystallinity of Pm3m and lattice parameter a = 0.3525 nm is a promising candidate for applications in electromagnetic devices [5].Among the studies previously done on fcc Fe-Ni alloys, those with a concentration of 65% Fe showed almost no thermal expansion at room temperature. It was observed that the other metallic systems also show the same unique invar behavior. Many researchers have conducted studies on some dynamic, thermodynamic and lattice magnetic properties of different important phases of Fe-Ni alloy such as $L12FeNi_3$, taenite L10FeNi and $L12Fe_3Ni$ using density functional theory method [6]. Also, 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 byseveral researchers. [7,8] using first principal DFT.The impetus of this work is to investigate the results of substituting an Mn and Cr atoms instead of a Ni atom in a $FeNi_3$ crystal. We then highlight the apparent differences in the results from the conventional $FeNi_3$ alloy crystal in each of the lattice parameters, band structures, density of states, magnetic parameters and optical properties.

2. Computational methodology

The first principles calculation of the ground state and electronic properties of $FeNi_3$ has been performed employing density functional theory using Siesta code [9] as a computational tool. The electronic configuration of Fe atom is [Ar] 4 s2 3d6, Ni atom is [Ar] 4 s2 3d8, Mnatomis [Ar] 4 s2 3d5 and Cr atom is [Ar] 4 s1 3d5. Exchange and correlation were chosen by the Perdew-Burke-Ernzerhof (PBE) [10] approach for calculation. All the computations incorporated in the present work are based on the Generalized Gradient Approximation (GGA). In order to calculate the structural, electronic and optical properties of $FeNi_3$, spin polarization and pseudo potential were used to represent the bonding relationship between ionic nuclei and electrons.

FCC phase of $FeNi_3$ has structure and is correspond to L21 structure of ternary Heusler alloys with the space group Pm3m. The unit cell of fcc $FeNi_3$ is shown in the Fig. 1, with four atomic bases: Fe (0, 0, 0), Ni_1(1/2, 0, 0), Ni_2(0, 1/2, 1/2), Ni_3(0, 0, 1/2).

The integration of the Brillouin zone was accomplished with 6 _ 6 _ 6Monkhorst-pack [11] k-point grid. The valence electron functions are expanded in a double zeta-polarizer basis set [12] of the local orbitals and the real space lattice is set to be 350 Ry. For the Hellmann-Feynman forces acting on all components of each atom to become smaller than0.005 eV/Å, the structure remains relaxed.

3. Results and discussion

3.1. Optimized Structures

Structural parameters of an originally relaxed $FeNi_3$ cell with a space group of Pm3m, in cores with four atoms defined by the following reduced coordinates: Fe (0, 0, 0) and three numbered for rested Ni atoms Ni_1 (1/2, 1/2, 0), Ni_2 (0, 1/2, 1/2), Ni_3 (1/2, 0, 1/2), the lattice constants of $FeNi_3$ alloy over the past decades have been verified many times, the basic structure of the stable $FeNi_3$ alloy is the $Pm\bar{3}m$ group structure and the lattice constants which is a = b = c = 3.528 Å, α = β = γ = 90.00°.Whereas in our present work, we find the lattice parameters for the new alloy $FeNi_2Mn$ is a = b = c = 3.551 Å, while alloy $FeNi_2Cr$ is a = b = c = 3.571 Å.

We based our calculations for this work on the Siesta code that was used to find the initial cell constants for $FeNi_3$alloys.After that, we replace one of the nickel atom with a manganese (Mn) atom the first time and a chromium (Cr) atom the second time to get the alloys $FeNi_2Mn$ and $FeNi_2Cr$. In this regard, the results have been compared with the data of the experiment and previous independent works, and we present in Table 1 the structural parameters of the primary $FeNi_3$ cell. We obtained that the lattice parameters of a $FeNi_3$, $FeNi_2Mn$ and $FeNi_2Cr$ (see Fig. 1).It was noted from Table 1 that the results reached are close to the previous theoretical and experimental work, and doping of the original compound $FeNi_3$with atoms of manganese (Mn) or chromium (Cr)changes the dimensions of the original cell and increases its size.

3.2. Electronic Properties

3.2.1 Structure of Energy

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.2 shows the Brillouin region of a cube. It is noteworthy that the study of properties in this region can be generalized later to FeNi2Mn and $FeNi_2Cr$. We used DFT theory and GGA approximation to determine the band gap of $FeNi_2Mn$ and $FeNi_2Cr$. This method has been relied upon because it is one of the most appropriate methods for studying the electronic structures of materials. The structure of energy bands of alloys is shown in Fig. 3.What can be seen in Figures 3a and 3b, where the highest valence bands overlap with the conduction bands, and this is evidence of the metallic property of the two alloys. We find that both alloys have ferromagnetic properties, with magnetic moments estimated to be values of 5.33μB and 5.47μB for $FeNi_2Mn$ and $FeNi_2Cr$, respectively.

3.2.2 Electronic Density of States (DOS)

We plotted both the total density of states (TDOS) and the partial density of states (PDOS) for $FeNi_2Mn$ and $FeNi_2Cr$ alloys using the GGA approximation and then analyzed them, 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 studied alloy, as shown in the fig. 4 and Fig. 5, respectively.Fig. 4 shows that the calculated TDOS for $FeNi_2Mn$and $FeNi_2Cr$ has high values with the GGA approximation in the region close to the Fermi level; we find that the TDOS value of $FeNi_2Cr$ is higher than that of $FeNi_2Mn$ and this indicates that its valence band is rich in electrons. In the region close to the Fermi level, we find that the highest peak density of states was recorded in $FeNi_2Mn$ alloy, which was estimated to be 4.34 (state/eV), while the value 4.06 (state/eV) was recorded as the highest value for $FeNi_2Cr$alloy.While we find exactly at the Fermi level that the largest value for the density of states was recorded at the$FeNi_2Cr$ alloy with a value estimated at: 2.58 (states/eV).

3.2.3. Partial Density of states (PDOS)

In this work, we have calculated and analyzed the partial density of states (PDOS) of $FeNi_2Mn$ and $FeNi_2Cr$ alloys in order to understand the movement of electrons close to the Fermi level. Figure 5a and 5b show the PDOS of $FeNi_2Mn$ and $FeNi_2Cr$ respectively.In the figure above, we present the density of incident states on atomic valence orbital (PDOS) in order to compare them with each other and also reveal the role of electrons in different atomic valence orbital, and how they affect the electronic properties. 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 iron and nickel atoms that make up the $FeNi_2Mn$ and $FeNi_2Cr$ alloys, we calculated the expected density of states throughout electron orbitals as a function of energy (E-EF).From the PDOS distributions, shown in Fig. 5a for the $FeNi_2Mn$ alloy, it can be shown that the electronic states are mainly located and substantially in the region of high activity, extending from -5 eV to +3 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;also, the contributions that come from the spin up Ni 3-d electrons are larger than those from the same spin down 3-d elements.The 3-d-orbitals terminal contribution of all atoms is also dominant inthe electronic distribution of $FeNi_2Mn$ and $FeNi_2Cr$ alloys.It is very clear from the two Figs. 5a and 5b that the manganese (Mn) or chromium (Cr) atoms added to the original $FeNi_3$alloy has added a lot in the electronic distribution in the region close to the Fermi level, and the alloy $FeNi_2Cr$ is considered the best in terms of chemical and catalytic activity from the alloy $FeNi_2Mn$.

3.3. Optical Properties

The study of the optical properties is very important, as its importance lies in obtaining information about the values of the optical constants of the material in a wide range of wavelengths. Based on this information, it can be used in the design and manufacture of optical blocks and optical pulses with different technologies uses.

3.3.1. Absorption coefficient

It expresses the decreasing ratio in the spectrum of the incident radiation energies with respect to the unit distance, in the direction of the direction of wave propagation within the medium. The absorption coefficient is related to the energy of the incident photons. Through it, the nature of electronic transitions can be known, and its equation is of the form:

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

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

The adsorption coefficient values for $FeNi_2Mn$ and $FeNi_2Cr$ alloys were calculated with approximations of GGA, and they are shown in Fig. 6.Fig.6 shows the change in the absorption coefficient as a function of the energy of the incident photon on the $FeNi_2Mn$ and $FeNi_2Cr$ alloys. From the figure it appears that the absorption coefficient in general begins to increase gradually with the increase in the energy of the photons of light, up to the value 3eV, it is also noted that three prominent peaks of the value of the absorption coefficient were recorded at the energies 2.91eV, 6.72 eV and 9.58 eV for $FeNi_2Mn$ alloy, and 3 eV, 6.92eV and 9.86 eV for $FeNi_2Cr$ alloy. In general, the behavior of both alloys in absorption is almost the same, except that higher values are recorded sometimes in the alloy $FeNi_2Cr$, this is especially when the amount of energy 1.86 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].

3.3.2. Optical Conductivity

It is a physical property that relates the current density to the electric field, and is given by the following equation:

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

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 $FeNi_2Mn$ and $FeNi_2Cr$ alloys were calculated with approximations of GGA, the results are as shown in Fig. 7.Fig.7 represents the photoconductivity changes in terms of the energy of photons falling on the $FeNi_2Mn$ and $FeNi_2Cr$alloys using the GGA approximations, in general, we notice that the value of photoconductivity increases with increasing energy of the two alloys, the values fluctuate between increasing at times and decreasing at other times, to record the highest value in the $FeNi_2Mn$ alloy the value 2465000 oum/cm^{-1}, while the highest value of the $FeNi_2Cr$ alloy reached the value 1143000 oum/cm-1.By comparing the two alloys, the $FeNi_2Mn$ alloy appears to be more optically conductive in the infrared and visible ranges. What can be concluded from the analysis of each of the absorption and optical conductivity curves is that $FeNi_2Mn$ and $FeNi_2Cr$ alloys have a good absorption value that allows their use in optoelectronics and photovoltaic compounds.

3.3.3. Refractive Index

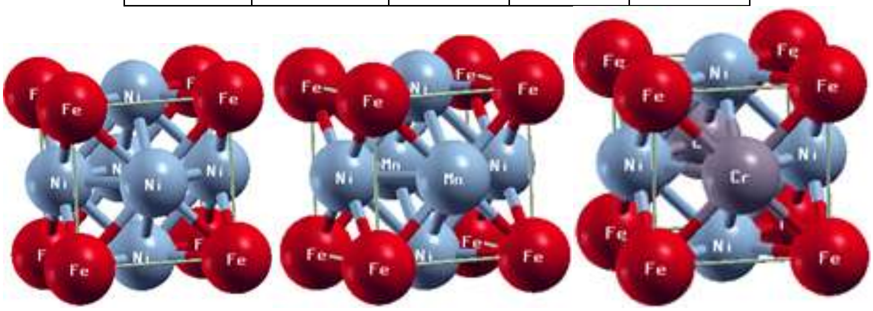
It is the ratio between the speed of light in free space and its speed in the matter, and the refractive index can be found according to the following equation:

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

The refractive index values for $FeNi_2Mn$ and $FeNi_2Cr$ were calculated using the GGA approximations as shown in Fig.8.By Fig.8, which expresses the refractive index in terms of incident photons, we noticed that the refractive indexn0 for the FeNi2Mn and FeNi2Cr are 28.5, 10.7 Respectively. Whereas, as the energy of the incident photons increased, the refractive index value began to decrease for both alloys, the value of the two alloys is approximately the same, starting from energy 0.5 eV. Also, the $FeNi_2Mn$ alloy is the one that has the largest value of the refractive index compared to the $FeNi_2Cr$ alloy.

Tabel 1. *Structural parameters of the optimized $FeNi_3$, $FeNi_2Mn$ and $FeNi_2Cr$ alloys and compared with theoretical and experimental result.*

	work	a (Å)	b (Å)	c (Å)
$FeNi_3$	Our work	3.528	3.528	3.528
	Theor[13]	3.548	3.548	3.548
	Exep[14]	3.55	3.55	3.55
$FeNi_2Mn$	Our work	3.551	3.551	3.551
$FeNi_2Cr$	Our work	3.571	3.571	3.571



(A) (B) (c)

Figure 1 *Structure of: (A) $FeNi_3$, (B)$FeNi_2Mn$, (C) $FeNi_2Cr$*

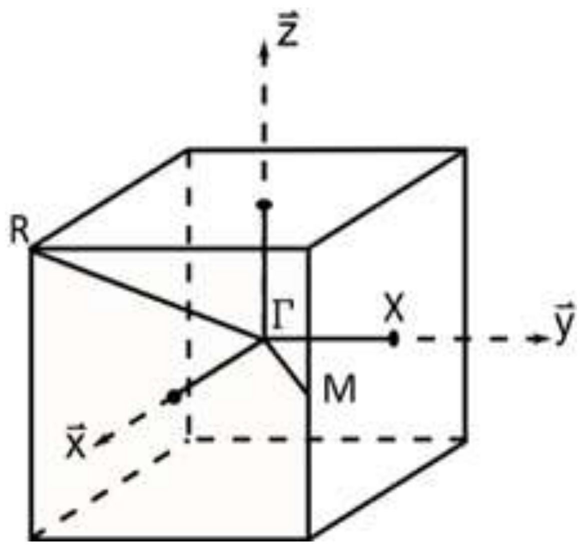


Figure 2 *Brillouin region of a cubic crystal*

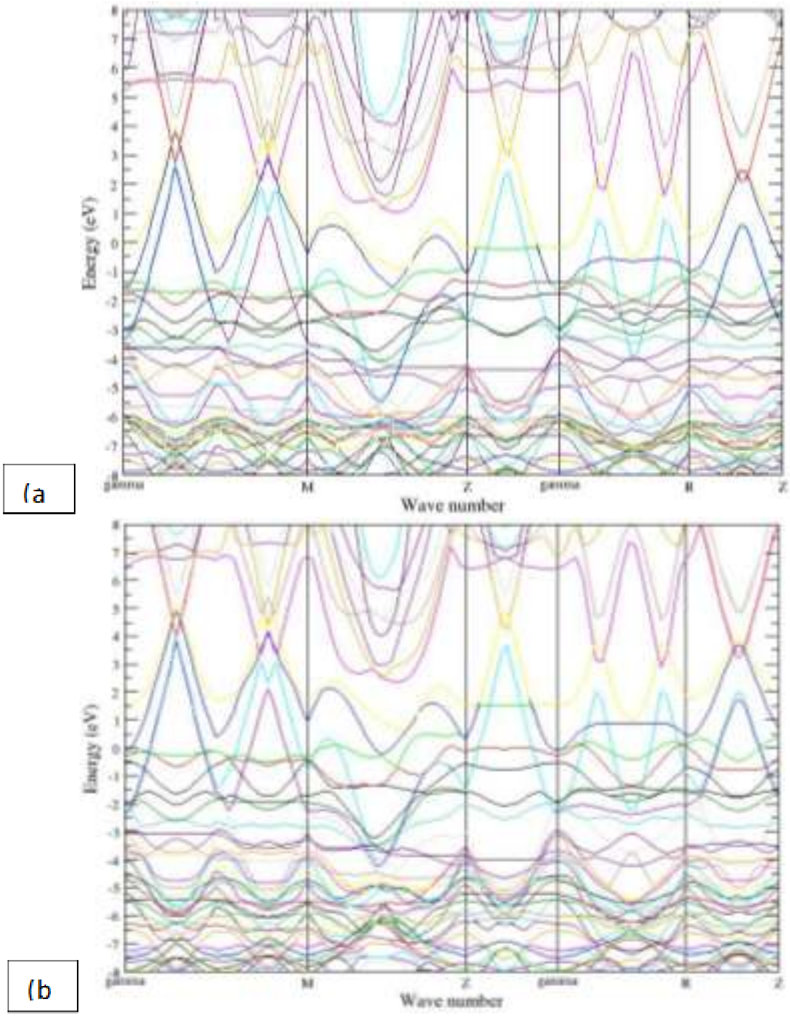


Figure 3 *– Energy bands structure of: (a) FeNi$_2$Mn, (b) FeNi$_2$Cr*

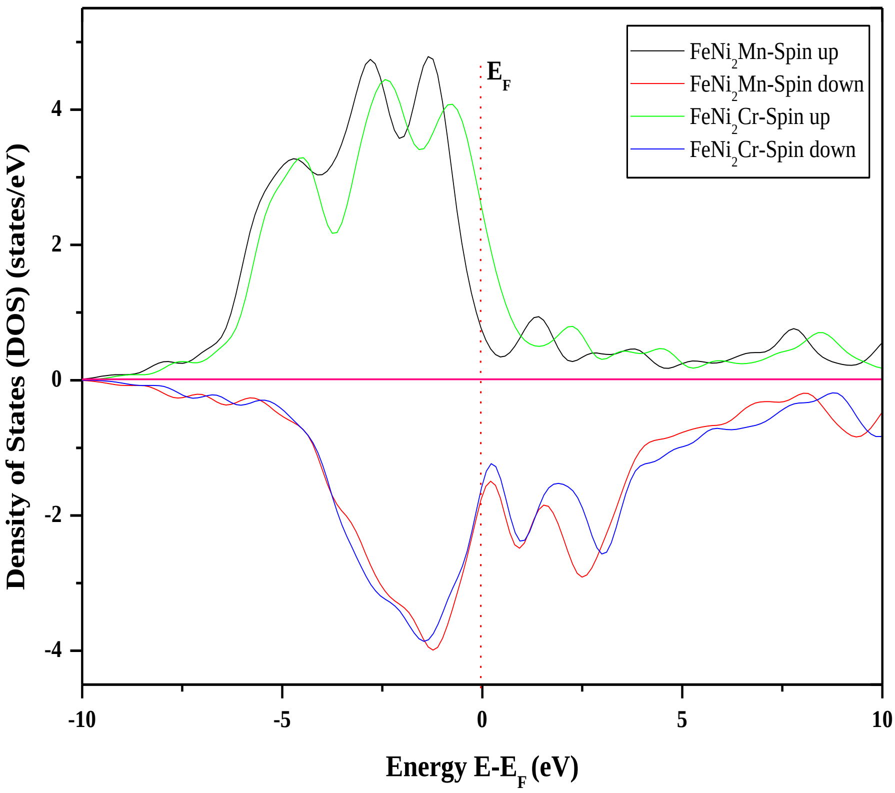


Figure 4 *Total density of states (TDOS) for:(a) FeNi$_2$Mn, (b) FeNi$_2$Cr*

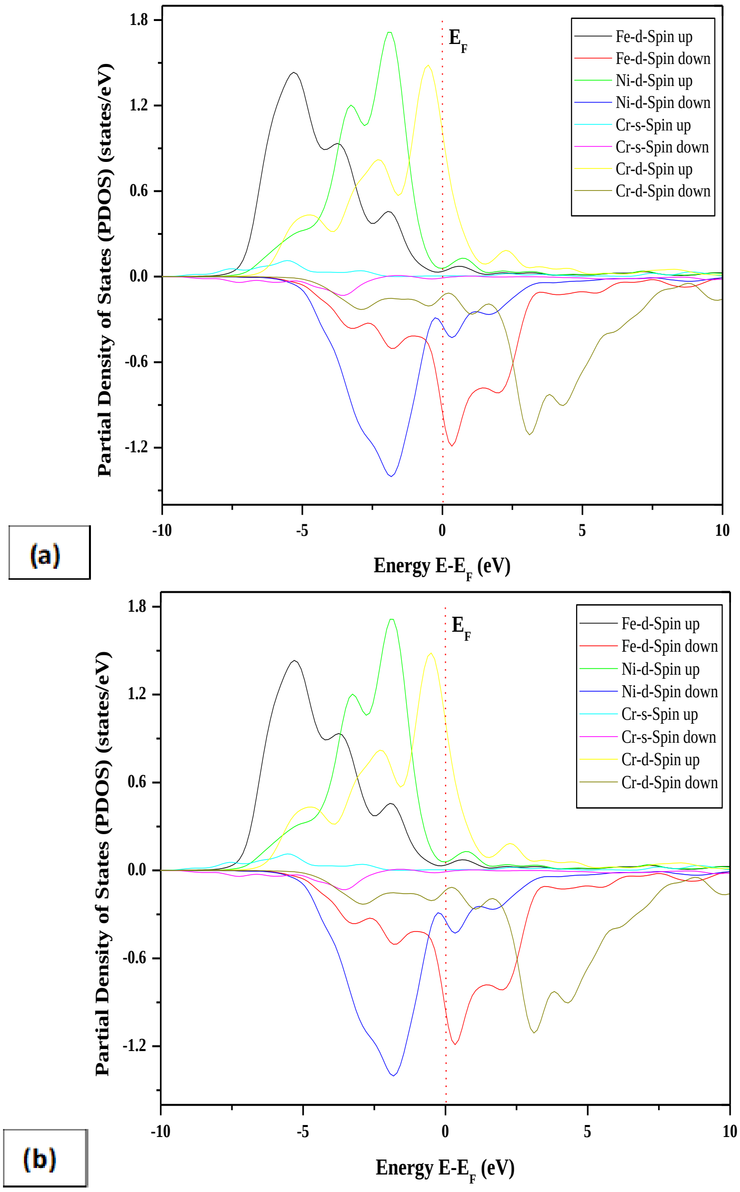


Figure 5 *Partial density of states (PDOS) for: (a) $FeNi_2Mn$, (b) $FeNi_2Cr$*

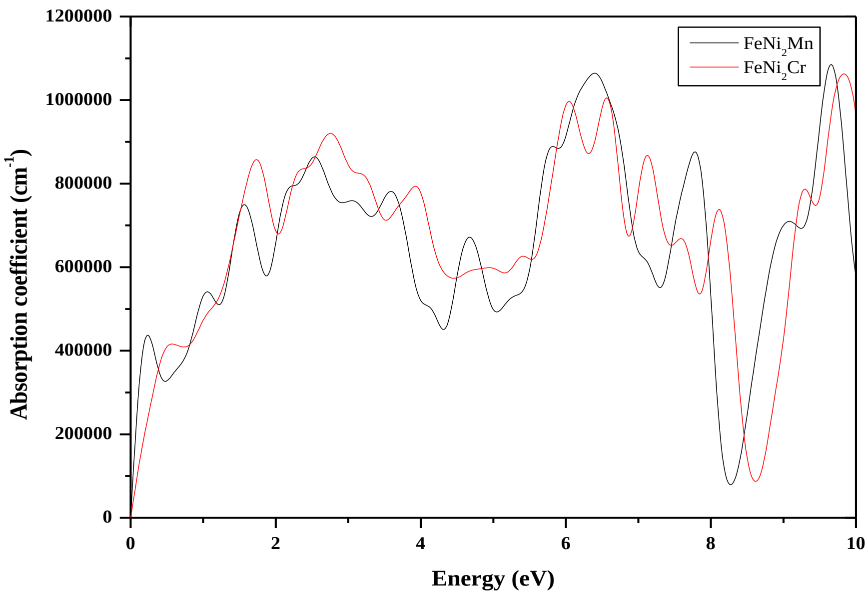


Figure 6 *Absorption coefficient of $FeNi_2Mn$ and $FeNi_2Cr$*

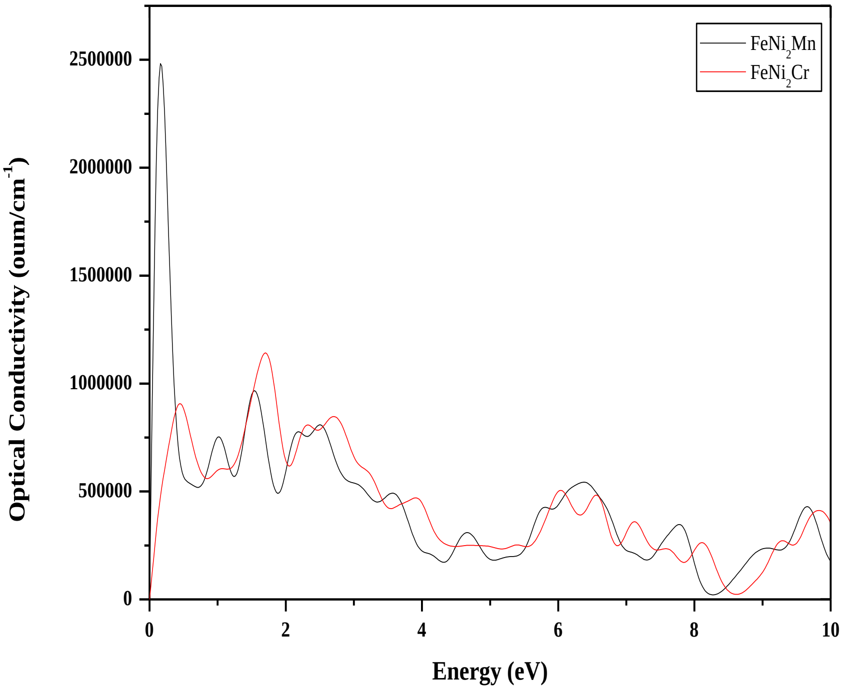


Figure 7 *Optical conductivity of $FeNi_2Mn$ and $FeNi_2Cr$*

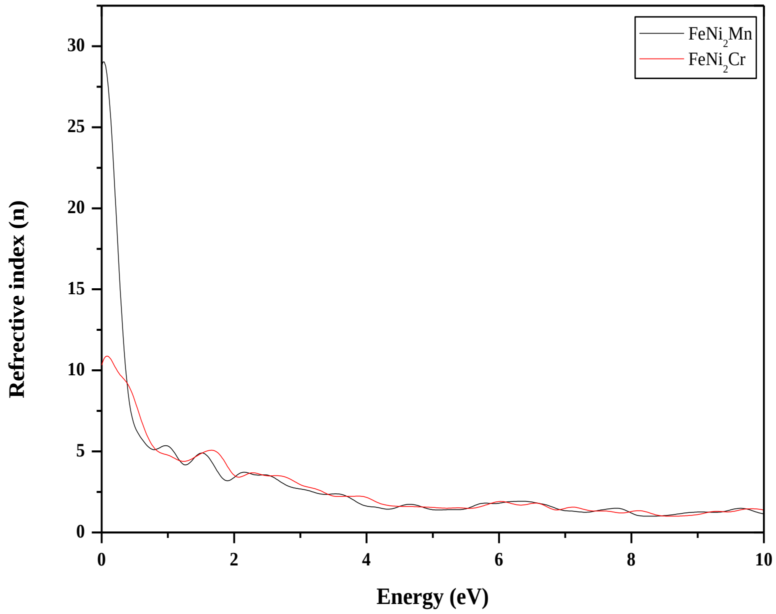


Figure 8 *Refractive index of $FeNi_2Mn$ and $FeNi_2Cr$*

4. Conclusions

Based on the calculations made according to the density function theory (DFT), and the use of the Siesta program, as well as the comparison of the results obtained through the alloys FeNi2Mn and FeNi2Cr, whether structural, electric or optical, to study the alloysFeNi2Mn and FeNi2Cr with fcc phase, it was concluded that:

- The structural parameters of the two alloys (FeNi2Mn and FeNi2Cr) are different from the structural parameters of the original alloy (FeNi3).
- Through the density of states, it was found that the two alloys have metallic properties, in addition to the FeNi2Cr alloy having a greater magnetic moment.
- From the comparison of the density of partial states recorded in the two alloys, it was found that the contribution of the orbiting 3 dis dominant and affecting the electronic and magnetic properties of the two alloys.
- Thanks to the differentiation in the optical properties of the two alloys, we find each has specific technological uses.

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
- **Conflict of interest:** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper

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- **Data availability statement:** The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

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