Effect of pressure on the geometric, electronic structure, elastic, and optical properties of the normal spinel MgFe$_2$O$_4$: a first-principles study

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Abstract

First-principles computation was used to study the effect of pressure on the elastic properties, magnetic properties, optical properties, and electronic structure of the normal spinel magnesium ferrite (MgFe$_2$O$_4$) at different pressures (0, 10, 20, 50, 70, and 100 GPa). The normal spinel MgFe$_2$O$_4$ has a direct bandgap of 1.62 eV which significantly decreased to 0.42 eV with increasing the pressure to 100 GPa. The values of the elastic constants were coherent with the mechanical stability norms for cubic crystals, which revealed that MgFe$_2$O$_4$ was mechanically stable. The values of Pugh’s ratio indicate that MgFe$_2$O$_4$ is ductile at all pressure values except at 100 Gpa MgFe$_2$O$_4$ shows brittle behavior. The computed values of the Zener anisotropy factor at different pressures were not equal to 1.0, which indicates that MgFe$_2$O$_4$ is elastically anisotropic. The optical properties (refractive index, reflectivity, dielectric function, optical conductivity, and loss function) for the normal spinel MgFe$_2$O$_4$, as well as its magnetic moment, were calculated and discussed at different pressures.

1. Introduction

Magnesium ferrite (MgFe$_2$O$_4$) is one of the most important spinel structured materials. It could be classified as $n$-type semiconductor direct bandgap [1] that can be used in several fields, such as hyperthermia [2], anode material [3], sensor [4], photocatalyst [5], and metal ion removal [6]. In addition to the easiness of preparation and low cost, MgFe$_2$O$_4$ has high resistivity, exhibits low dielectric, and magnetic losses [7]. Spinel ferrites are important ceramics with various and interesting optical, magnetic, structure, and electronic properties. The general formula of spinels is AB$_2$O$_4$. The spinels have a cubic crystal structure adopting the space group Fd$ar{3}$m. They have eight formula units for each unit cell. They consist of thirty-two O anions in close packing cubic in addition to twenty-four cations. Spinels can be classified according to the occupation of metal ions on the tetrahedral and the octahedral sites into normal spinel and inverse spinel. In the normal spinel, the 8 divalent cations occupy the tetrahedral sites and all sixteen trivalent cations occupy the octahedral ones. In the inverse spinel, the 16 octahedral sites are equally divided between 8 divalent and 8 trivalent cations, while the remaining 8 trivalent cations occupied the tetrahedral sites [8]. Most studies on MgFe$_2$O$_4$ have focused on the experimental part while few of them are interested in the theoretical part. Maensiri et al [9] have reported that MgFe$_2$O$_4$ has a cubic structure of normal spinel-type and is a soft magnetic $n$-type semiconducting material. Guo et al [10] have used density functional theory (DFT) the first systematic study of diverse MgFe$_2$O$_4$ surfaces in three types of spinel structures: normal, mixed, and inverse. Guo et al [11] have studied the contribution from diverse facets of three spinel systems of MgFe$_2$O$_4$, normal-spinel, mixed-spinel, and inverse-spinel. Boukokkeze et al [12] have investigated the structural, optical, elastic, and electrical properties of spinel LiZn$_2$Fe$_3$O$_8$ nanoparticles annealed at two distinct temperatures. Boukokkeze et al [13] have investigated the structural, optical, elastic, and electrical
properties of spinel LiZn$_2$Fe$_3$O$_8$ nanoparticles annealed at two distinct temperatures. Pawar et al [14] have studied inter-atomic bonding and dielectric polarization in Gd$^{3+}$ incorporated Co-Zn ferrite nanoparticles.

Our previous study has shown the effect of vacancies on the geometric structure, electronic structure, the optical properties, and magnetic properties of MgFe$_2$O$_4$. The crystal structures of the Fe-vacancy and O-vacancy defects distorted from the perfect cubic crystal structure, whereas the deformation of the Mg-vacancy structure was negligible. All the structures with vacancy defects could not be formed spontaneously; however, O-vacancy was the easiest to form, followed by Fe-vacancy and Mg-vacancy under specific conditions. The bandgap of MgFe$_2$O$_4$ with Mg-vacancy and Fe-vacancy defects have the properties of half-metallic ferromagnets materials, and they could be promising materials for spintronic device applications [15]. The novelty of this work is the assumption of normal spinel structure of the ferrite under investigation. Additionally, it is the first study of the pressure effect of the mechanical, electronic, optical and magnetic properties under applied pressure at extreme conditions. In this work, we have focused on the effect of pressure on the geometric structure, electronic structure, the elastic properties, magnetic properties, and the optical properties of the normal spinel MgFe$_2$O$_4$.

2. Computational details

The normal spinel magnesium ferrite (MgFe$_2$O$_4$) with Fd$3m$ space group was used, in which Wyckoff positions were 8a for magnesium atoms, 16d for iron atoms, and 32e for oxygen atoms [15]. Spin-polarized density functional calculations were carried out with the help of the Cambridge Serial Total Energy Package (CASTEP) program [16, 17], with the use of a total energy plane-wave pseudopotential method [18]. The revised Perdew–Burke–Ernzerhof (RPBE) [19] functional of the generalized gradient approximation (GGA) was used to explain the exchange and correlation interaction among electrons. The Brillouin zone of the structures was sampled with 2 × 2 × 2 k-point of Monkhorst–Pack. The energy cut off was 380 eV. The convergence criteria of geometry optimization of the largest force on atoms were 0.01 eV Å, and the self-consistent convergence accuracy was set at 5 × 10$^{-6}$ eV/atom, respectively. These calculations were carried out with Hubbard-U correction (GGA + U) [20], where the 3$d$ orbitals for the Fe atoms were treated with a U value of 5.0 eV. Our previous study concluded that $U = 5.0$ eV was the optimum value for MgFe$_2$O$_4$ [15].

The elastic constants were calculated at different pressures (0, 10, 20, 50, 70, and 100 GPa). The number of steps for each strain was 4, and the maximum strain amplitude was 0.003 eV/atom. The calculations were carried out with convergence tolerance as follows: energy = 1.0 × 10$^{-6}$, maximum force = 0.002 eV Å, and the maximum displacement = 1.0 × 10$^{-4}$ Å. The elastic modulus matrix for the cubic crystal system can be written as:

$$[C_{ij}] = 
\begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{12} & 0 & 0 & 0 \\
\varepsilon_{12} & \varepsilon_{11} & \varepsilon_{12} & 0 & 0 & 0 \\
\varepsilon_{12} & \varepsilon_{12} & \varepsilon_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & \varepsilon_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & \varepsilon_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & \varepsilon_{44}
\end{bmatrix}$$

A cubic crystal has only 3 various elastic constants $\varepsilon_{11}$, $\varepsilon_{12}$ and $\varepsilon_{44}$. The elastic constants fulfill the mechanical stability standards [21] if verifying the following relation:

$$\varepsilon_{11} > 0, \varepsilon_{44} > 0, \varepsilon_{11} > |\varepsilon_{12}|, (\varepsilon_{11} + 2\varepsilon_{12}) > 0$$

(1)

The values of Young’s modulus (E) and Poisson’ ration (v) could be computed from equations (2) and (3),

$$E = \frac{9BG}{3B + G}$$

(2)

$$V = \frac{3B - 2BG}{2(3B + G)}$$

(3)

The value of the Zener anisotropic factor (A) could be computed from equation (4) [22],

$$A = \frac{2\varepsilon_{44}}{(\varepsilon_{11} - \varepsilon_{12})}$$

(4)

The optical functions of normal spinel MgFe$_2$O$_4$ at different pressures (0, 10, 20, 50, 70, and 100 GPa) were calculated with [100] polarization vector. We have used a 0.5 eV smearing for all calculations. The complex dielectric function is one of the basic optical properties of a solid, which is calculated from equation (5),

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

(5)
In CASTEP, the real part $\varepsilon_1(\omega)$ could be computed from the Kramers-Kroning relationship [23], while the imaginary part $\varepsilon_2(\omega)$ of the dielectric constant is computed numerically by including direct assessment of the matrix elements among the occupied and unoccupied electronic states.

3. Results and discussion

3.1. Structural properties

Figure 1 displays the lowest-energy structure of normal spinel MgFe$_2$O$_4$. The computed lattice parameters, Mulliken population, and bond lengths (Å) for normal spinel MgFe$_2$O$_4$ at different pressures were reported in Table 1. The computed lattice parameters were decreased with increasing the pressure. From Table 1, the computed bond lengths of Mg–O, Fe–O, and O–O were decreased with increasing the pressure. Herein, the pressure affected the unit cell volume and therefore leads to enhanced densification.

| Pressure (GPa) | $a=b=c$(Å) | Atom  | Charge(e) | Bond  | Population | Bond length(Å) |
|---------------|-------------|-------|-----------|-------|------------|----------------|
| 0             | 8.71        | Mg    | 1.66      | Mg–O  | −0.88      | 2.036          |
|               |             | Fe    | 1.00      | Fe–O  | 0.30       | 2.094          |
|               |             | O     | −0.91     | O–O   | −0.04      | 2.834          |
| 10            | 8.70        | Mg    | 1.65      | Mg–O  | −0.87      | 2.040          |
|               |             | Fe    | 1.00      | Fe–O  | 0.30       | 2.091          |
|               |             | O     | −0.91     | O–O   | −0.04      | 2.825          |
| 20            | 8.38        | Mg    | 1.84      | Mg–O  | −1.47      | 1.935          |
|               |             | Fe    | 0.96      | Fe–O  | 0.33       | 2.028          |
|               |             | O     | −0.94     | O–O   | −0.05      | 2.767          |
| 50            | 8.14        | Mg    | 0.37      | Mg–O  | −1.92      | 1.872          |
|               |             | Fe    | 0.45      | Fe–O  | 0.35       | 1.977          |
|               |             | O     | −0.32     | O–O   | −0.05      | 2.705          |
| 70            | 7.92        | Mg    | 0.35      | Mg–O  | −2.56      | 1.799          |
|               |             | Fe    | 0.43      | Fe–O  | 0.38       | 1.934          |
|               |             | O     | −0.30     | O–O   | −0.06      | 2.666          |
| 100           | 7.74        | Mg    | 0.34      | Mg–O  | −3.03      | 1.745          |
|               |             | Fe    | 0.42      | Fe–O  | 0.41       | 1.897          |
|               |             | O     | −0.30     | O–O   | −0.06      | 2.627          |

In CASTEP, the real part $\varepsilon_1(\omega)$ could be computed from the Kramers-Kroning relationship [23], while the imaginary part $\varepsilon_2(\omega)$ of the dielectric constant is computed numerically by including direct assessment of the matrix elements among the occupied and unoccupied electronic states.

3.2. Elastic properties

The values of the elastic constants were listed in Table 2. From table 2, the elastic constants fulfill the mechanical stability standards [22] given by equation (1). It implies that the examined spinel structure is mechanically stable under the studied pressures range. To further examine the mechanical properties of the magnesium ferrite, the
bulk modulus \( (B) \) and shear modulus \( (G) \) could be achieved from Voigt-Reuss-Hill averaging scheme \([23]\) by using the values of calculated elastic constants. From table 2, the values of bulk modulus \( (B) \) are higher than the values of shear modulus \( (G) \) at different pressures, which illustrates that the \( G \) parameter restricts the mechanical stability. The increase in the bulk modulus with increasing the pressure is directly correlated with decreasing the compressibility \([24]\). This trend agrees with the decrease in the lattice parameter and bond lengths. The ratio between the tensile stress and the tensile strain is defined as Young’s modulus \( (E) \), which is a significant parameter that can be used for measuring the stiffness of the material. As \( E \) increased the solid become stiffer \([24]\). From table 2, the values of computed \( E \) increases as the pressure increases slightly till 20 GPa and then decreases with further increase pressure. We can say that the stiffness is in a direct relationship with the pressure till 20GPa. From the above discussion, it is clear that the pressure has a deep effect on the stiffness of MgFe\(_2\)O\(_4\). The Poisson’s ratio measures the stability of the material; its value is proportional to the plasticity of materials. Furthermore, Poisson’s ratio presents information that is beneficial in the characteristic of the bonding forces. Nye has reported that if the value of Poisson’s ratio between (0.50–0.25) the solid has central force \([25]\). From table 2, the values of computed Poisson’s ratios at different pressures are higher than 0.25 (the value of the lower limit), which indicates that the interatomic force in MgFe\(_2\)O\(_4\) is the central force. It is obvious as the spinel structure is centrosymmetric and possesses the highest crystal symmetry in its cubic form. Pugh’s ratio \( (B/G) \) is an important parameter for differentiation between the ductile and brittle behavior of a solid \([22]\). If the value of Pugh’s ratio is higher than 1.75, the material has ductile behavior, while if the value of Pugh’s ratio is less than 1.75 the material has a brittle behavior. From table 2, all the values of Pugh’s ratio at the different pressures are higher than 1.75 except at 100GPa, this indicates that MgFe\(_2\)O\(_4\) is ductile at all pressure values and transforms to brittle at 100 GPa. The values of anisotropic factor \( (A) \) enable us to differentiate between elastically isotropic and elastically anisotropic materials. If the value of \( A \) is 1.0 the material is elastically isotropic, other than that the material is elastically anisotropic. From table 2, the computed values of Zener anisotropy factors \( (A) \) at different pressures are not equal to 1.0, which indicates that MgFe\(_2\)O\(_4\) is elastically anisotropic. Herein, the anisotropy along the lattice cube side differs than that along the body diagonal of the spinel matrix as also the number of ions in that direction.

### Table 2. Computed elastic constants \( (c_{11}, c_{12}, c_{44}) \) GPa, bulk modulus \( (B, \text{GPa}) \), shear modulus \( (G, \text{GPa}) \), Young’s modulus \( (E, \text{GPa}) \), Poisson’s ration \( (\gamma) \), Pugh’s ratio \( (B/G) \) and anisotropic factor \( (A) \) at different pressure for MgFe\(_2\)O\(_4\).

| MgFe\(_2\)O\(_4\) (GPa) | \( c_{11} \) | \( c_{12} \) | \( c_{44} \) | \( B \) | \( G \) | \( E \) | \( \gamma \) | \( B/G \) | \( A \) |
|-------------------------|---------------|---------------|---------------|-------|-------|-------|-------|-------|-------|
| 0                       | 180.93        | 104.49        | 80.47         | 129.97| 63.57 | 163.98| 0.28  | 2.04  | 0.69  |
| 10                      | 181.01        | 104.63        | 80.58         | 130.09| 63.62 | 164.12| 0.28  | 2.04  | 0.70  |
| 20                      | 181.23        | 104.71        | 80.72         | 130.22| 63.73 | 164.39| 0.28  | 2.04  | 0.70  |
| 50                      | 287.19        | 251.13        | 80.67         | 263.00| 55.61 | 155.86| 0.40  | 4.72  | 3.21  |
| 70                      | 326.17        | 412.98        | 69.14         | 384.04| 24.12 | 70.89 | 0.46  | 15.92 | −5.06 |
| 100                     | 353.21        | 541.58        | 57.36         | 478.79| −3.25 | −9.78 | 0.50  | −147.3| −5.1  |

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**Figure 2.** The relation between lattice parameter \( (a) \) and bulk modulus (reciprocal of compressibility) at different pressures.
3.3. Electronic properties

The computed band structures of the normal spinel MgFe$_2$O$_4$ at different pressures (0–100) GPa are shown in figure 3. It clearly shows that the MgFe$_2$O$_4$ is a direct bandgap semiconductor with a bandgap of 1.62 eV. From table 3 the bandgap values were decreased with increasing pressure. As the pressure increases, the volume of the crystal decrease, bond-length decreases, and the interatomic distance decreases as shown in table 1, which enhances the re-distribution of electron density and encourage a high covalency. Lattice materials are portrayed by their equivalent elastic moduli for investigating mechanical properties of the microstructures. The estimations of the elastic moduli under static forcing condition are essentially reliant on the geometric properties of the unit cell and the mechanical properties of the intrinsic material. Under a static forcing condition, the equivalent elastic moduli (e.g., Young’s modulus) are always positive. When dynamic forcing is considered, the equivalent elastic moduli turn to a function of the applied frequency and they could be negative at certain frequency values [26]. At this extremely high pressure values 100 GPa, we could probably ascribe the negative values to a large deformation in the ferrite. This could be the focus of our future to build up an experimental setup to study the effect of pressure on the physical properties of the ferrite materials.

Figure 3. The band structure of MgFe$_2$O$_4$ at 0 GPa (a), 10 GPa (b), 20 GPa (c), 50 GPa (d), 70 GPa (e) and 100 GPa (f); spin-up states (black lines), spin-down stated (red line).
Figure 4 shows the computed spin-polarized partial density of states (PDOS) and the total density of states (TDOS) of MgFe$_2$O$_4$ within the GGA + U framework. The position of the Fermi energy level is specified by the dashed vertical line, which belongs to the energy of zero. From figure 4 it is clear that near the Fermi level the density of states belongs to O 2p state and Fe 3d state. Furthermore, the 3d orbitals (electrons) of Fe are the basic contributor to the conduction band minimum (CBM). The 3d of Fe and 2p of O are the basic contributor to the

Figure 4. The calculated total and partial density of states of the normal spinel MgFe$_2$O$_4$ at different pressure values.
valence band maximum (VBM). This illustrates the presence of a covalence bond between O and Fe atoms. We can observe the matching of these results with that reported in table 1 of the Mulliken population. It is well-known that a large value of the bond population denotes a covalent bond, while a low value indicates the ionic bonds. A value of zero denotes a perfectly ionic bond and the values higher than zero denote the increasing levels of covalency \[27\]. Table 1 shows that the values of Mulliken overlap populations of Fe–O bond. Fe–O bond has a covalent character, and as the pressure increases the strength is of the bond increase. By the inspection of the TDOS near to the Fermi level, it was found that the states of the CBM were shifted toward the Fermi level, while the states of the VBM were unchanged, and this explains the decreasing of the bandgaps with increasing the pressures. In general, all spin-up and spin-down states were shifted away from the Fermi level except for the Mg-2p states at \(-39.0\) to \(-41.0\) eV.

### 3.4. Effect of pressure on the magnetic moment of normal spinel MgFe$_2$O$_4$

The total magnetic moment ($M_{\text{total}}$, $\mu_B$) of normal spinel MgFe$_2$O$_4$ calculated at different pressures per formula unit is listed in table 4. The magnetic moments were calculated via Hirshfeld analysis \[28\]. The calculated magnetic moment for the Fe ion at 0 GPa was 4.16 $\mu_B$, and this value was decreased with increasing the pressure as follows: (4.15, 4.13, 4.09, 4.06 and 4.02) $\mu_B$ for (10, 20, 50, 70, and 100) GPa, respectively. A lot of experimental results reported that Fe ion has a high spin-state in ferrites \[29, 30\]. The magnetic moment, which resulted from the unpaired electrons in an atom, could be used in describing the Fe charge state \[29\]. It has been reported that the magnetic moments were 4.23 $\mu_B$ for the Fe$^{3+}$ in LaFeO$_3$, 3.61 $\mu_B$ for the Fe$^{4+}$ in SrFeO$_3$ and 3.92 $\mu_B$ for Fe$^{3.5+}$ in La0.5Sr0.5FeO$_3$ \[22\], respectively. Thus, the observed decrease in the magnetic moments of the normal spinel MgFe$_2$O$_4$ as the pressure increased could be attributed to changes in the valence of some Fe ions. Furthermore, if the charge on Fe changes, the Fe–O adopting a high charge and the bond length should then decrease. The Fe–O bond length was decreased from 2.094 Å to 1.897 Å as the pressure decreased from 0 GPa to 100 GPa, indicating that the Fe charge changes (table 1). Additionally, as the pressure increases the porosity will decrease. Porosity is a microstructure that is very important in a magnetic material, as it can affect the process of shifting the domain walls during magnetization that would affect to magnetic properties. Furthermore, as the pressure increase the volume of the unite cell decrease, large positive pressure effect caused by a redistribution of the spin-polarized electronic states as their hybridization changes under pressure. Another possible influence of the pressure is the decrease in the bond lengths as clarified in table 1, which directly vary the exchange interaction between Fe ions through the intervening oxygen cations. Herein, the system will be transformed into short range order rather than long range one. We could not neglect a small canting due to deviation of the spin order from perfect collinearity at higher pressures.

| Pressure (GPa) | $M_{\text{total}}$ ($\mu_B$) | Integrated spin density/ cell unit | Integrated spin density/ cell unit |
|---------------|-----------------|----------------------------------|----------------------------------|
| 0             | 9.98            | 80.00                            | 80.026                           |
| 10            | 10.00           | 80.00                            | 80.028                           |
| 20            | 10.02           | 80.00                            | 80.017                           |
| 50            | 10.03           | 80.00                            | 80.006                           |
| 70            | 10.02           | 80.00                            | 80.009                           |
| 100           | 9.99            | 80.00                            | 80.008                           |

### Table 3. Computed band gap of the normal spinel MgFe$_2$O$_4$ at different pressures.

| Pressure (GPa) | Band gap (eV) |
|---------------|---------------|
| 0             | 1.62          |
| 10            | 1.57          |
| 20            | 1.40          |
| 50            | 1.18          |
| 70            | 0.77          |
| 100           | 0.42          |

### Table 4. Total magnetic moment ($M_{\text{total}}$, $\mu_B$), integrated spin density($\mu_B$), and integrated |spin density| ($\mu_B$) of MgFe$_2$O$_4$ at different pressures.

| Pressure (GPa) | $M_{\text{total}}$ ($\mu_B$) | Integrated spin density/ cell unit | Integrated spin density/ cell unit |
|---------------|-----------------|----------------------------------|----------------------------------|
| 0             | 9.98            | 80.00                            | 80.026                           |
| 10            | 10.00           | 80.00                            | 80.028                           |
| 20            | 10.02           | 80.00                            | 80.017                           |
| 50            | 10.03           | 80.00                            | 80.006                           |
| 70            | 10.02           | 80.00                            | 80.009                           |
| 100           | 9.99            | 80.00                            | 80.008                           |
The magnetic states of normal spinel MgFe₂O₄ at different pressures can be illustrated from the integrated spin density and the absolute value of integrated spin density (table 4). If both values of the integrated spin density and the absolute value of integrated spin density are non-zero and equal, the material is considered ferromagnetic. From table 4 we can note that normal spinel MgFe₂O₄ at different pressures is ferromagnetic.

### 3.5. Optical properties

Figure 5 presents the reflectivity spectra of the normal spinel MgFe₂O₄ as a function of photon energy calculated at different pressures. The reflectivity values at 0.01 eV at 0, 10, 20, 50, 70, and 100 GPa are 0.11, 0.16, 0.11, 0.16, 0.25, and 0.34, respectively. The reflectivity at 70 and 100 GPa dropped sharply in the infrared region and reached a minimum at ~1.0 eV, while at 10 and 50 GPa was increased and a sharp peak located in the ultraviolet region at ~4.08 eV was observed. Some peaks were observed for all pressures from 10–30 eV. The reflectivity drops again in the ultraviolet region for all pressures starting from ~31 to 45 eV. Some sharp peaks in the region of ~46–67 eV were observed in this region. The peak values are seen to be proportional to the pressure value. In general, as the pressure increases the height of the peak increases and shifted to higher energies. Figure 6 shows the computed absorption spectra of normal spinel MgFe₂O₄ at different pressures, which revealed that the absorption spectra occurs in (1 to 25) eV and (46 to 62) eV regions. This indicates that the MgFe₂O₄ absorption band covering a large range of the ultraviolet and visible regions. Additionally, MgFe₂O₄ at 0, 20, 70, and 100 GPa has an absorption peak below 1 eV. Therefore, it is expected that MgFe₂O₄ could be promising
photocatalysts. The MgFe$_2$O$_4$ being used as a photocatalyst in visible light owing to its small bandgap [31]. The most important factor of the photocatalysis process is optical absorption. A considerable small bandgap will result in increased the absorption of light. The absorption peaks increased with increasing the pressure which could be attributed to the decrease of the bandgap. The optical conductivity is a significant parameter that resulted from the transition of the electrons in the occupied states to unoccupied states above the Fermi level when absorbing photon energy.

Figure 7 represents the calculated real part of optical conductivity and the imaginary part of optical conductivity for normal spinel MgFe$_2$O$_4$ at different pressures. It is clear from this figure that both the real and imaginary parts of optical conductivity were increased as the pressure increased. The optical conductivity peaks reached its maximum height at 100 GPa, where the real optical conductivity reached 35.68 at 57 eV. The observed slight shifting towards the high energy with increasing pressure could be attributed to the decrease in the bandgaps.

Figure 8 illustrates the real parts and imaginary parts of the dielectric functions up to 70 eV. The real dielectric values at 0.01 eV at 0, 10, 20, 50, 70, and 100 GPa were 3.90, 5.58, 3.96, 5.29, 8.83, and 13.15, respectively. This indicates that increases the pressure enhanced the normal spinel MgFe$_2$O$_4$ polarization. It can be noted that the first optical critical point (real part) appears near 2.5–3.0 eV which belongs to 10 and 50 GPa, then rapidly drops around 5.0 eV. There are several peaks in two regions of 0.7 to 17 eV and 45 to 61 eV. The height of these peaks was increased and shifted toward high energies with increasing the pressure. The first peaks of the imaginary part of the dielectric function appear in the region of 0.5 to 25 eV, and then gradually decreases to zero around 25 to 48 eV. Other peaks of $\varepsilon_2(\omega)$ appear in the range of 45 to 62 eV. The observed shifting in energies with the increase in pressure is not only attributed to the decrease in the band length. This in turn increased the net dipole moment as the pressure increase.

The refractive index presents the amount of light is curved, or refracted, during entering a material [32]. The refractive indices of the normal spinel MgFe$_2$O$_4$ at different pressures are shown in figure 9. The static refractive index values of normal spinel MgFe$_2$O$_4$ at 0, 10, 20, 50, 70, and 100 GPa are 1.97, 2.36, 1.99, 2.30, 2.99, and 3.66, respectively. From these values, we can note that the static refractive indices at high pressures are greater than
that of at 0 GPa. The highest static refractive index was observed at 100 GPa. The static refractive indices at different pressures were in the infrared region and gradually shifted in the visible region and ultraviolet region.

The electron energy loss function is an important optical parameter. Figure 10 shows the energy loss function of normal spinel MgFe$_2$O$_4$ at different pressures. In describing the loss of energy at the different pressures, the prominent peaks found at different pressures are responsible for a collective oscillation of the electrons in the valance band. This is shown in figure 10. Such a peak is located at different frequencies for different pressures. At this frequency, the real part of the dielectric tensor of the different pressures is going through zero. The electron loss is found to be small and firmly reflected in the UV region.

4. Conclusions

In this paper, we studied the structural, elastic, electronic, magnetic, and optical properties of normal spinel MgFe$_2$O$_4$ at various pressures using DFT. The results showed that the lattice parameters and bond lengths decreased with increasing the pressure. The bandgap values were decreased with increasing the pressure. The elastic constants fulfill the mechanical stability standards for cubic crystals. All the values of bulk modulus ($B$) are higher than the values of shear modulus $G$ at different pressures, which illustrates that ($G$) restricts the mechanical stability. The computed Poisson’s ratio indicated that the interatomic force in MgFe$_2$O$_4$ is the central force at the different pressures. The values of Pugh’s ratio ($B/G$) indicated that MgFe$_2$O$_4$ has ductile behavior at (0–70 GPa), while at 100 GPa MgFe$_2$O$_4$ has brittle behavior. The computed values of the Zener
anisotropy factor indicated that MgFe$_2$O$_4$ is elastically anisotropic at different pressures. The calculated bandgaps decreased with increasing the pressure. From studying the magnetic properties, MgFe$_2$O$_4$ showed ferromagnetic behavior at different pressures. For the optical functions (reflectivity, absorption, optical conductivity, dielectric functions, refractive index, and loss function) of normal spinel MgFe$_2$O$_4$, the peaks, in general, were increased and were shifted toward to high energy. In our future work, we aimed to explore what could happen experimentally after discussing the results of the computational studies to better understand the physics of magnetic materials under extreme conditions.

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