Structural and optical properties of sol-gel synthesized h-MoO$_3$ nanorods treated by gamma radiation

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Abstract

High energy external gamma radiation has always an impact on semiconductor material by altering its physico-chemical properties. In this paper, the effect of gamma-radiation is observed on sol-gel synthesized metastable h-MoO$_3$ nanorods with absorbed dose variation. The irradiated sample shows a remarkable change in their structural parameters such as average crystallite size decreased, strain, and dislocation density increased and so on are confirmed from the x-ray diffraction (XRD). Functional groups and the corresponding vibration and stretching are analyzed from the Fourier transform infrared spectroscopy (FTIR). The change in surface morphology is observed from the field emission scanning electron microscopy (FESEM) image and found no remarkable change. However, the optical band gap decreases with increasing absorbed dose and calculated 2.84 eV, 2.82 eV, 2.80 eV and 2.77 eV for 0 kGy, 40 kGy, 80 kGy, and 120 kGy, respectively by Kubelka-Munk function from the diffuse reflectance data of UV–vis-NIR spectrophotometer.

1. Introduction

At present, transition metal oxide is a key topic in the research arena as it can produce different phases by changing the metal–oxygen ratio, and MoO$_3$ has become an attractive candidate among others due to its structure dependent electrical and optical properties variation [1]. MoO$_3$ is a wide bandgap (2.8–3.6 eV) semiconductor with n-type conductivity [2, 3]. Good stability under ambient conditions and wide bandgap make MoO$_3$ a potential applicant for high power transistor and transparent conducting layer application in optical components [4, 5]. Moreover, literature shows several industrial applications of MoO$_3$ such as gas sensors, anode in lithium-ion batteries and high reactive photocatalysts because of their electro-chemical and chromogenic properties [6–8].

Crystallite MoO$_3$ has commonly three polymorphic structures; one stable orthorhombic ($\alpha$-phase), and two metastable phases namely hexagonal ($h$-phase) and monoclinic ($\beta$-phase), respectively [4, 7, 9]. Even, the difficulties of metastable phase synthesis and to keep its property stable, hexagonal phase attracts more attention among other phases. Moreover, 1D behavior of h-MoO$_3$ with tunneling structure shows some dominant physical and chemical properties [8].

Metastable hexagonal MoO$_3$ remains stable in its phase up to 410 °C $\sim$ 436 °C and after further temperature increment, a permanent irreversible ($\alpha$-phase) phase transition may occur [3, 10]. Phase stability is an important concern for optoelectronic and photonic device application. Phase stability may be interrupted by several external influences such as temperature, pressure, physico-chemical behavior and also the ionizing and non-ionizing radiation [11]. Simchi et al shows that the efficiency of Cu(InGa)Se$_2$ thin film solar cells with MoO$_3$ back contact decreased after annealing at higher temperature due to phase transformation from hexagonal to
orthorhombic [12]. Almodóvar et al [13] reported that non-ionizing red laser (633 nm) radiation changes metastable hexagonal to the orthorhombic MoO$_3$ phase without further morphological modification. However, Sen et al[14] observed that gamma radiation as ionizing radiation has no impact on phase transformation of MoO$_3$ while structural, optical and electrical properties are significantly changed by absorbing gamma photon.

The scientific community paid special attention to the impact of gamma radiation on metal oxide semiconductor (MOS) as it creates a partial distortion in semiconductor’s structure that leads to electrical and optical characteristics variation. Generally, the effect of radiation on a material depends upon its position from the source, irradiation time and the types of radiation sources such as neutrons, gamma, electron, and ions, etc [15]. Depending upon the energy of gamma photon three possible phenomena may occur in a matter. Sufficient energy of gamma irradiation can change the physical properties of MOS by creating structural defects like vacancies (oxygen vacancy) or dislocation due to ionization and/or atomic displacements which is the basis for an increment of charge carrier density [16, 17].

Literature survey shows that gamma radiation has significant impacts on the technological applications of MOS based devices due to the modification of their physico-chemical properties. Chandoul et al studied the low energy gamma radiation effect on a-MoO$_3$ nanorod thin films prepared by spray pyrolysis [17]. Sen et al shows that the optical bandgap changes due to the dose variation of hydrothermally synthesized a-MoO$_3$ nanoplates [16]. There were several experiments carried out to understand the influence of gamma radiation on other transition metal oxides such as ZnO nanowire, nanopowder, and Mg-doped shows a decrement of optical band gap after irradiation [18–20]. S kaya et al shows that oxygen vacancies increase in Er$_2$O$_3$ but don’t change its physical properties significantly after irradiation [21]. Gas sensing property of SnO$_2$ enhances with the radiation dose increment however, a higher dose can create a large number of oxygen vacancies [22, 23].

Previously, we investigated the gamma radiation effects on thin films of hexagonal phase of molybdenum trioxide (h-MoO$_3$) fabricated by thermal spray pyrolysis and Doctor Blade methods. In those works considerable changes were observed on the structural and optical characterizations of both types of thin films [14, 24]. In this present work, we examined the impact of the total absorbed dose of gamma radiation on the sol-gel synthesized metastable hexagonal MoO$_3$ nanoparticles with rod-like shape. The phase confirmation and crystallographic analysis of pristine and irradiated samples were investigated with x-ray diffraction (XRD) technique. The field emission scanning electron microscopy (FESEM) and UV–vis spectroscopy were used to determine the surface morphology and optical characteristics, respectively. The functional groups were identified with the Fourier transform infrared spectroscopy (FTIR) analysis.

2. Experimental detail

2.1. Materials and methods

To synthesize hexagonal molybdenum trioxide nanoparticle by sol–gel method, all the chemical reagents were purchased in analytical grade from Sigma Aldrich, and no further purification was done. For the synthesis of hexagonal MoO$_3$, the precursor was ammonium heptamolybdate tetrahydrate (AHM) [(NH$_4$)$_6$Mo$_7$O$_{24}$·4H$_2$O] and 67% concentrated HNO$_3$.

0.2 M aqueous solution of ammonium heptamolybdate tetrahydrate (AHM) [(NH$_4$)$_6$Mo$_7$O$_{24}$·4H$_2$O] was prepared by dissolving 2.32 g in 10 ml of deionized water. The solution was stirred for 30 min in a magnetic stirrer at a constant rotation speed. A concentrated nitric acid (67% HNO$_3$) of 5 ml was added dropwise into the solution at room temperature. After that, the solution was heated in a water bath at 85 °C for 4 h and a white color precipitation was observed. The solution was kept in a dark room at 25 °C temperature for a week. The residues were washed several times with acquis solution of ethanol and the centrifuge precipitated MoO$_3$ was dried in a vacuum oven at 75 °C for 4 h.

2.2. Gamma (γ) irradiation

As-synthesized h-MoO$_3$ nanopowder samples were irradiated with a commercial Cobalt-60 gamma irradiator source of 63.54 kCi in the Institute of Food and Radiation Biology (IFRB), Atomic Energy Research Establishment (AERE), Bangladesh Atomic Energy Commission. Before irradiation, a liquid phase dosimetry (Ceric-cerous system) was done by placing a dummy sample 25.4 cm away from the source and the calculated absorbed radiation rate was 12.17 kGy h$^{-1}$ [20]. Therefore, the h-MoO$_3$ samples were irradiated for different time intervals to get the absorbed doses 40 kGy, 80 kGy, and 120 kGy respectively.

2.3. Characterization tools

The crystalline and phase identification of the pristine and irradiated h-MoO$_3$ samples were investigated by x-ray diffraction (model 3040–X’Pert PRO) from CuKα source of wavelength 1.541 78 Å with a scanning rate of 1° min$^{-1}$ at room temperature. The surface morphology was observed by the high-resolution image of the Field
Emission Scanning Electron Microscope (FESEM) (Model: JEOL JSM-7600F) with 5 kV accelerating voltage. Functional group and phase stability studies were carried out by using Fourier Transform Infrared Spectroscopy (FTIR) (Model: FTIR-ATR Perkin Elmer Spectrum Two) in the wavenumber range 4000–400 cm$^{-1}$. The optical bandgap was measured from the UV–vis-NIR spectroscopy (Model: PerkinElmer UV-Vis_NIR spectrometer Lambda 1050) data using the reflected spectra in the range of wavelength 200–800 nm.

3. Result and discussion

3.1. Morphology study
Figure 1 shows the micrographs ($\times$ 30,000) of pristine and gamma-irradiated h-MoO$_3$ nano-particle samples with different absorbed doses of 40 kGy, 80 kGy, and 120 kGy. FESEM image shows MoO$_3$ nanorods were successfully synthesized. The inset photo of the as-synthesized pristine sample shows 1D hexagonal nanoroads with a diameter of about $\sim$150 nm which proves the legitimacy of XRD data. Nanorods were a solid bar in different sizes and irregularly distributed. The flower-like substances are the agglomerated crystal of h-MoO$_3$. However, surface morphology shows no significant changes after gamma irradiation with different doses.

3.2. Crystallographic structure analysis
The powder X-ray diffraction (XRD) patterns of pristine and gamma irradiated sample of MoO$_3$ nanoparticle is shown in figure 2. The XRD experiment was carried out from 5$^\circ$ to 70$^\circ$ at 2$\theta$ position with CuK$_{\alpha}$ ($\lambda = 1.54056$ Å) radiations. The diffracted peaks are well indexed with the hexagonal phase of molybdenum trioxide (h-MoO$_3$) according to the JCPDS-21-0569 data card (lattice parameters $a = 10.53$ Å and $c = 14.97$ Å, space group no P63)$^2$, $^{25}$. The major identified peaks such as (100), (110), (200) and (210) of pristine sample reveal the poly-crystal in nature and the absence of any additional peaks of impurity or secondary phases of MoO$_3$ namely orthorhombic or monoclinic indicates the purity of hexagonal phase. After gamma photon irradiation on pristine h-MoO$_3$, the...
number of distinguishable diffracted peaks remains unchanged, but a substantial variation is observed in the case of both peak intensity and position.

The highest intense peak is observed for plane (210) at the diffracted angle of 25.7° which indicates the preferential orientation for pristine sample. Moreover, the major peak remains unchanged in the plane (210) after absorbing gamma photon. The intensity of (210) peak gradually decreased with the increase of total absorbed dose of gamma radiation as shown in figure 2 (inset). During initial interaction of nanostructured MoO$_3$ with gamma photon of absorbed dose 40 kGy, the intensity of major peak (210) is decreased sharply. Further increase of absorption doses at 80 kGy and 120 kGy the peak intensity remains declined, but the intensity reduction rate was lower. This may be due to the crystal imperfections or re-arrangement in crystal structure of MoO$_3$. The peak intensity depends on the scattering factor that attributed to the number of electrons per atom in the crystal lattice [24]. However, ionization due to gamma irradiation produces more or less electron. Moreover, Yoshio et al [26] explained that other several factors such as crystal structure modification, absorption factor, polarization factor, Lorentz factor, and temperature factors are responsible for peak intensity variation. Thus, it is clear that all these factors may participate in XRD peak intensity variation. The peak intensity decrement indicates the deterioration in crystallinity [27]. Many research reports claimed that the point defect due to the oxygen vacancies leads to the reduction of crystallinity with an increasing total absorbed dose of gamma radiation [21, 23, 28].

The position of the prominent peak shifted towards the left side of 2θ value from 25.77° to 25.68° after exposing with a higher absorbed dose at 120 kGy. Lattice strain, defects formation in the crystal structure, and variation in inter-planar distance may cause the XRD peak shifting. Chithambararaj et al [8] reported that the presence of strain in the lattice structures may change the inter-planar distance that leads to the peak position shifting. Here, the inter-planar spacing of h-MoO$_3$ increases from 3.452 Å to 3.461 Å for the (210) plane after exposed pristine sample with 120 kGy.

This inter-planer spacing increment implies the defect generation and the compressive strain increment resulting from the micro-stress in the nanocrystal material owing from the lattice vibration due to the local heat generation after radiation absorption [1, 21, 29]. The calculated parameters in table 1 clearly reveals the argument.

Average crystallite size, dislocation density, and lattice strain were determined for (100), (110), (200) and (210) planes presented in table 1. The well-known Debye–Scherrer’s formula was used to determine the crystallite size ($D$) of h-MoO$_3$ nanoparticles [30] as follows

$$D = \frac{K \lambda}{\beta_{hkl} \cos \theta_{hkl}}$$

Where, $\beta_{hkl}$ represents the XRD peak broadening at half maximum intensity of the respective (hkl) plane, $\theta_{hkl}$ defines the Bragg diffraction angle (in degrees), $\lambda$ is the wavelength of x-ray source ($\lambda = 1. 54056$ Å for CuK$_{\alpha}$),
| Dose (kGy) | Peak (hkl) | 2θ (deg.) | FWHM (deg.) | Crystallite Size, D (nm) | D_{ave} (nm) | Strain (ε) ($\times 10^{-4}$) | ε_{ave} ($\times 10^{-4}$) | Dislocation Density, δ ($\times 10^{14}$ lines/nm$^2$) | δ_{ave} ($\times 10^{14}$ lines/nm$^2$) |
|-----------|------------|-----------|-------------|-------------------------|-------------|-------------------------------|------------------|---------------------------------|---------------------------------|
| 0         | (100)      | 9.70      | 0.1316      | 63.28                   | 48.10       | 67.60                         | 52.92            | 2.50                            | 4.72                            |
|           | (110)      | 16.83     | 0.1847      | 45.41                   | 54.49       | 4.85                          | 5.10             | 6.44                            |                                  |
|           | (200)      | 19.43     | 0.1901      | 44.30                   | 48.43       |                               |                  |                                 |                                  |
|           | (210)      | 25.78     | 0.2159      | 39.42                   | 41.17       | 6.44                          |                  |                                 |                                  |
| 40        | (100)      | 9.59      | 0.136 81    | 60.86                   | 47.24       | 71.13                         | 54.27            | 2.70                            | 4.84                            |
|           | (110)      | 16.71     | 0.1796      | 46.69                   | 53.36       | 4.58                          | 5.57             | 6.53                            |                                  |
|           | (200)      | 19.31     | 0.198 79    | 42.33                   | 50.97       |                               |                  |                                 |                                  |
|           | (210)      | 25.68     | 0.217 61    | 39.10                   | 41.64       | 6.53                          |                  |                                 |                                  |
| 80        | (100)      | 9.63      | 0.129 97    | 64.06                   | 51.25       | 67.29                         | 49.95            | 2.43                            | 4.15                            |
|           | (110)      | 16.74     | 0.156 51    | 53.58                   | 46.40       | 3.48                          |                  |                                 |                                  |
|           | (200)      | 19.35     | 0.1773      | 47.47                   | 45.37       | 4.43                          |                  |                                 |                                  |
|           | (210)      | 25.71     | 0.213 19    | 39.92                   | 40.75       | 6.27                          |                  |                                 |                                  |
| 120       | (100)      | 9.63      | 0.1474      | 56.47                   | 45.26       | 76.36                         | 56.56            | 3.14                            | 5.145                           |
|           | (110)      | 16.74     | 0.1873      | 44.78                   | 55.55       | 4.99                          |                  |                                 |                                  |
|           | (200)      | 19.35     | 0.2019      | 41.69                   | 51.67       | 5.75                          |                  |                                 |                                  |
|           | (210)      | 25.72     | 0.2233      | 38.11                   | 42.69       | 6.88                          |                  |                                 |                                  |

Table 1. Structural parameter modification with gamma irradiation dose variation of h-MoO$_3$. 


and the value of shape factor is 0.94. The average crystallite size decreases from 48.15 nm of pristine sample to 47.24 nm for a lower absorbed dose of 40 kGy and after then increases to 51.25 nm for 80 kGy. Further increase of absorption dose at 120 kGy the crystallite size again decreases and shows lower value than 40 kGy doses, detail in table 1. Crystallite size variation does not show a gradual patter but it seems a declining trend with absorbing dose increment. Here, at the initial stage of absorbing dose, it may be expected that the local heat is generated due to the interaction of MoO3 crystal with high energy gamma photon which consequently occurs atomic displacement and/or ionization [31]. When applied gamma photon interacts with synthesized molybdenum trioxide nanomaterial of hexagonal structure, it transfers the kinetic energy into the lattice points of the crystal that generates lattice vibration and micro-stress. This leads lattice phonon scattering, which creates local heating [21, 31]. However, the crystal size decrement is an indication of poor crystallinity after irradiation.

The tensile stress that makes the d spacing larger due to inhomogeneous strain, observed from the peak shifting is an indication of structural defects like interstitial dislocations, vacancies, and layer faults claim a clear defect formation in the h-MoO3 nanoparticle after gamma irradiation. However, the value of average crystallite size of h-MoO3 after irradiation become close to the reported value of Chithambararaj et al [8]. The average lattice strain (ε) was calculated by utilizing the Stokes–Wilson equation [32] as
\[
\varepsilon = \frac{\beta_{hkI}}{4 \tan \theta_{hkI}}
\]

Dislocation density is also an important parameter to detect the crystallinity and its value augmentation in this research work after γ-irradiation, designates the displacement of atoms with respect to reference-lattice positions, and this may be due to the heat generation and lattice vibration in the molecular bond [21, 33]. Smaller the dislocation density, the better the crystal structure. However, the larger dislocation density implies a higher hardness [16, 27]. The average dislocation density increases from $4.72 \times 10^{14}$ to $5.14 \times 10^{14}$ lines/nm² after irradiated pristine sample with a gamma photon absorption dose of 120 kGy.

Dislocation density (δ) was determined by the following equation [34]
\[
\delta = \frac{1}{D^2}
\]

Where, D is the average crystallite size. Thus, the overall structural study reveals that with increasing gamma irradiation dose, the structural parameter changed remarkably by decreasing the crystallinity without an immense change its crystal orientation. A comparison of previous and present study on structural and optical properties variation of MoO3 after gamma irradiation with different doses prepared in different methods in table 2.

| Dose (kGy) | Synthesis Method | Pristine phase | Phase change after irradiation | Crystallite size (nm) | Band gap (eV) | References |
|------------|------------------|----------------|-------------------------------|----------------------|---------------|------------|
| 0          | Spray pyrolysis  | α-MoO3 nanorod thin films | No | 105.62 | 3.92 | [17] |
| 0.1        |                  |                |                               | 109.32 | 3.93 | |
| 10         |                  |                |                               | 105.74 | 3.89 | |
| 50         |                  |                |                               | 104.46 | 3.96 | |
| 30         | Spray pyrolysis  | h-MoO3 thin films | No | 65.56 | 3.00 | [14] |
| 60         |                  |                |                               | 64.81 | 3.07 | |
| 90         |                  |                |                               | 60.72 | 3.14 | |
| 120        | Doctor blade     | h-MoO3 thin films | No | 58.48 | 3.20 | |
| 50         | Hydrothermal     | α-MoO3 nanoplates | No | 46.00 | 2.92 | [24] |
| 150        |                  |                |                               | 51.77 | 2.90 | |
| 250        |                  |                |                               | 55.28 | 2.88 | |
| 300        |                  |                |                               | 59.13 | 2.84 | |
| 10          | Hydrothermal     | α-MoO3 nanoplates | No | 135.31 | 2.78 | [16] |
| 120        |                  |                |                               | 127.79 | 2.85 | |
| 40          | Sol gel          | h-MoO3 nanorods | No | 136.00 | 2.90 | |
| 80          |                  |                |                               | 48.10 | 2.84 | This research work |
| 120        |                  |                |                               | 47.24 | 2.82 | |
| 120        |                  |                |                               | 51.25 | 2.80 | |
| 120        |                  |                |                               | 45.26 | 2.77 | |

3.3. Functional group study
To analyze the functional groups and phase stability, FTIR spectra are graphically represented in figure 3 in the range of 400 to 4000 cm⁻¹ for nonirradiated (0 kGy) and irradiated (40 kGy, 80 kGy, 120 kGy) samples.

Table 2. Comparison of structural and optical properties of different phases MoO3 after gamma irradiation prepared in different method.
respectively. A small peak at 3217 cm$^{-1}$ of stretching and an obvious vibrational peak at 1614 cm$^{-1}$ was spotted as a common characteristic feature of OH groups of adsorbed surface water. The N–H group of ($\text{NH}_4^+$) ions shows bending and stretching vibrational at 3072 cm$^{-1}$ and 1416 cm$^{-1}$ respectively. The origin of the N–H bending and stretching vibrations from the N-H group of ammonium ions ($\text{NH}_4^+$) evolved due to the application of precursor material ammonium heptamolybdate tetrahydrate ($\text{AHM}$) [($\text{NH}_4$)$_6\text{Mo}_7\text{O}_{24}.4\text{H}_2\text{O}$]. A significant change is observed in hydrogen bonded OH and NH groups vibration after gamma absorption dose variation. The OH group vibration increases with $\gamma$- irritation indicates the lengthening and weakening of H-O-H bonds.

Two strong stretching peaks for Mo=O bond were observed at the 861 cm$^{-1}$ and 685 cm$^{-1}$ wavenumbers for the pristine sample and shows no remarkable variation after $\gamma$- dose absorption. However, a high transmitted peak for Mo–O vibration was observed at 575 cm$^{-1}$ shifted to 578 cm$^{-1}$ after dose variation. The small deviation in the transmitted peak intensity and position of stretching and bending vibrations of Mo=O, Mo–O bond indicates the defect formation, and it may be due to the small local heat generation by means of irradiated dose absorption variation. The full FTIR experimental data is depicted in table 3.

### Table 3. Functional group analysis of h-MoO$_3$ nanorods with different doses.

| Functional group                              | Wavenumber (cm$^{-1}$) |
|----------------------------------------------|------------------------|
|                                              | 0 kGy  | 40 kGy  | 80 kGy  | 120 kGy |
| H–O–H stretching vibration                   | 3217   | 3556    | 3536    | 3221    |
| N–H stretching vibration                     | 3072   | 3044    | 3105    | 3069    |
| H–O–H bending vibration                      | 1614   | 1610    | 1622    | 1617    |
| N–H bending vibration                        | 1416   | 1414    | 1414    | 1414    |
| Mo=O stretching vibration                    | 861, 685 | 861, 697 | 861, 686 | 862, 683 |
| Mo–O vibration                               | 575    | 578     | 578     | 574     |

Figure 3. FTIR spectra of gamma irradiated h-MoO$_3$ nanoparticles.

3.4. Optical absorbance study

UV visible spectra analysis is a key technique to understand the electrical structure of a semiconductor. Figure 4 shows the comparison of diffuse reflectance spectra of nonirradiated and irradiated samples observed from 200 to 800 nm wavelength at room temperature. The graph shows that at the 40 kGy the diffuse reflectance spectra increases and for further increase of absorption dose of 80 kGy and 120 kGy the reflectance decreases gradually. This indicates that at the initial lower dose the stoichiometry was improved while imperfection in crystallinity of h-MoO$_3$ occurred for further gamma absorption dose increased. The maximum reflectance was observed in the visible range of 420 nm to 500 nm wavelength.
As the optical band gap cannot measure directly from the spectrophotometer, the absorption coefficient of the sample was calculated by the Kubelka-Munk (K-M) function from diffuse reflectance spectra and the band gap was determined from the Tauc plot shown in figure 5. The K-M function is given as

$$ F(R) = \frac{K(\lambda)}{S(\lambda)} = \frac{(1 - R)^2}{2R} $$

Where $F(R)$ is the K-M function, $K(\lambda)$ is the absorption coefficient, $S(\lambda)$ is the scattering coefficient, and $R$ indicates the diffuse reflectance.

However, $F(R)$ is proportional to the absorption coefficient as the scattering coefficient can be considered a constant for our experimental wavelength. Thus,

$$ F(R) \propto \alpha = \frac{(h\nu - E_g)^n}{h\nu} $$

Where $h\nu$ is the incident photon energy, $E_g$ is the band gap. For the direct band gap the value of power factor $n = 1/2$. The optical band gap was measured from the linear region of the plot of $[F(R) \times h\nu]^2$ versus incident photon energy ($h\nu$). The calculated optical band gap for 0 kGy, 40 kGy, 80 kGy, and 120 kGy samples are 2.84 eV, 2.82 eV, 2.80 eV, and 2.77 eV respectively shown in figure 5.
The optical band gap decrement with the absorbed dose increment indicates the formation of crystal defects, i.e. disorder or vacancies in h-MoO₃ nanoparticles. During the interaction of gamma with the matter, some atoms in the nanoparticle can be removed causing a point defect. This crystal defect created localized states in the band gap thus, the Fermi level-shifted towards the conduction band and this state act as a recombination center [36, 37]. Therefore, conductivity increases by lowering the optical band gap of the nanoparticle. Kamari et al [36] reported that with increasing gamma irradiation dose, the density of states increased which attributes the increment of an absorption coefficient, subsequently shifting the absorption edge towards the lower energies and reduced the band gap. In this experiment, the band gap of h-MoO₃ decreased with increasing irradiation dose may be due to the cause of defect generation by creating oxygen vacancies that leads the localized state generation in the nanoparticle. Arshak et al [38] also mentioned that crystal defect due to gamma irradiation was mostly oxygen vacancies and in some cases distortion in the stoichiometry of its structure.

4. Conclusion

This research work was designed to understand the influence of gamma irradiation on metastable hexagonal MoO₃ nanoparticle with absorb dose (0 kGy, 40 kGy, 80 kGy, and 120 kGy) variation and finally confirmed about its impact by studying some structural and optical properties. The XRD pattern shows both peaks shifted about 2θ about 25.77° to 25.68° for (210) plane, and peak broadening (about 0.18° to 0.19°) after irradiated the pristine sample with a higher absorbed dose of 120 kGy. The average crystallite size was calculated 48.15 nm 47.24 nm, 51.25 nm, and 45.26 nm for the absorption dose variation from pristine to higher doses respectively. The average strain increases 54.92 × 10⁻⁴ to 56.56 × 10⁻⁴ and dislocation density increases from 4.72 × 10¹⁴ to 5.14 × 10¹⁴ lines/nm² after irradiated pristine sample with a gamma photon absorption dose of 120 kGy. The functional group analysis shows that the metal oxide bond (Mo=O, Mo-O) stretching and vibration peak position changes with increasing irradiation dose. The micrograph analysis was carried out by the FESEM image and shows no remarkable variation in its morphology after irradiation. However, the optical band gap decreased gradually from 2.84 eV to 2.77 eV for every step of irradiation dose increment that was calculated from the diffuse reflectance data of UV–vis-NIR spectrophotometer.

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